CONTEMPORARY MATHEMATICS

640

Spectral Theory and Partial Differential Equations

Conference in honor of James Ralston's 70th Birthday
Spectral Theory and Partial Differential Equations
June 17–21, 2013
University of California, Los Angeles, Los Angeles, California

Gregory Eskin
Leonid Friedlander
John Garnett
Editors

American Mathematical Society

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To Jim Ralston on the occasion of his seventieth birthday

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Preface

This volume's authors participated in the Conference in Spectral Geometry and Partial Differential Equations that took place at UCLA on June 17–21, 2013. Both the conference and the volume are dedicated to Jim Ralston on the occasion of his 70th birthday. Jim is well known for his work in PDEs, spectral theory, and inverse problems. Through his ideas, and his support and encouragement of young mathematicians, Jim has made a great contribution to the field.

We would like to thank the speakers at the conference, all of the participants, the authors of this volume, and the referees. Their effort made the conference a success and allowed this volume to appear. Lastly, the conference was partially supported by the NSF grant DMS1301620.

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John Garnett

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Algebras in reconstruction of manifolds

M. I. Belishev

Abstract. The paper is an extended version of the talk given at the Conference in UCLA dedicated to the jubilee of J.Ralston. The subject is applications of some ideas of noncommutative geometry to inverse problems on manifolds with boundary. We show that the boundary inverse data determine the C*-algebras, whose topologized spectra are identical to the manifold. By this, to recover the manifold is to determine a relevant algebra from the inverse data, find its spectrum, and endow the spectrum with a Riemannian structure.

0. Introduction

We deal with two dynamical systems associated with a Riemannian manifold with boundary. The first one is a system governed by the scalar wave equation, the second is governed by the Maxwell equations. Both of the systems are controlled from the boundary. The inverse problems are to recover the manifold via the relevant measurements at the boundary (inverse data).

We show that the inverse data determine the C*-algebras, whose (topologized) spectra are identical to the manifold. By this, to recover the manifold is to determine an appropriate algebra from the inverse data, find its spectrum, and provide the spectrum with a Riemannian structure.

The paper develops an algebraic version [**2**], [**4**] of the *boundary control method*, which is an approach to inverse problems based on their relations to control theory [**1**], [**3**]. The most promoted and detailed exposition of the version see in [**6**].

1. Setup

1.1. Acoustics. Let Ω be a compact connected smooth[1] Riemannian manifold with the boundary Γ, $\dim \Omega = n \geqslant 2$; Δ is the (scalar) Beltrami-Laplace operator on Ω.

In the paper, all the functional spaces, classes, and algebras are*real*.

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Key words and phrases. Reconstruction of manifolds via boundary inverse data, C^*-algebras, boundary countrol method.

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[1]everywhere in the paper, "smooth" means C^∞-smooth

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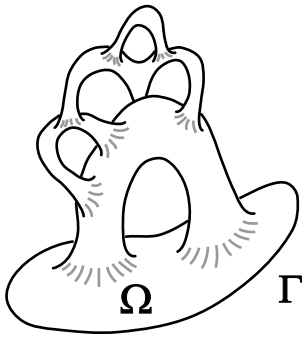

FIGURE 1. Manifold

Forward problem of acoustics is to find a solution $u = u^f(x,t)$ of the system

$$u_{tt} - \Delta u = 0 \qquad \text{in } (\Omega\backslash\Gamma)\times(0,T) \tag{1.1}$$

$$u|_{t=0} = u_t|_{t=0} = 0 \qquad \text{in } \Omega \tag{1.2}$$

$$u = f \qquad \text{on } \Gamma\times[0,T]\,, \tag{1.3}$$

where $f \in \mathcal{F}^T := L_2(\Gamma\times[0,T])$ is a (given) *boundary control*.

With the system one associates a *response operator* $R^T : \mathcal{F}^T \to \mathcal{F}^T$,

$$R^T f := u^f_\nu\big|_{\Gamma\times[0,T]}\,,$$

where ν is the outward unit normal to Γ, $(\,)_\nu := \frac{\partial}{\partial\nu}$. This operator is well defined on smooth controls vanishing near $t = 0$.

Inverse problem is: *given for a fixed* $T >$ diam Ω *the operator* R^{2T}, *to recover* Ω.

The meaning of the condition $T >$ diam Ω and time doubling (the use of R^{2T}) is of kinematic nature. The external observer prospects the manifold by acoustical waves initiated at the boundary. The waves propagate with velocity 1. By the latter, the waves must be given enough time to travel through the manifold, accumulate information about its interior structure, and return back to the boundary, where they are detected by the observer.

1.2. Electrodynamics. In addition to the previous assumptions on Ω, let it be *oriented*, $\dim\Omega = 3$. We adhere standard definition and notation of the vector analysis operations $\wedge$, curl , div on a $3d$-manifold: see, e.g., [**11**], Chapter 3.

Forward problem is to find a solution $e = e^f(x,t)$, $h = h^f(x,t)$ of the Maxwell system

$$e_t = \operatorname{curl} h,\ h_t = -\operatorname{curl} e \qquad \text{in } \Omega\times(0,T) \tag{1.4}$$

$$e|_{t=0} = 0,\ \ h|_{t=0} = 0 \qquad \text{in } \Omega \tag{1.5}$$

$$\nu\wedge e = f \qquad \text{in } \Gamma\times[0,T]\,, \tag{1.6}$$

where $f \in \mathcal{F}^T := L_2([0,T];\vec{L}_2(\Gamma))$ is a *boundary control* (time-dependent tangent field on Γ).

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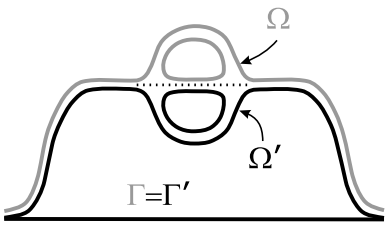

FIGURE 2. Nonuniqueness

With the system one associates a *response operator* $R^T : \mathcal{F}^T \to \mathcal{F}^T$,

$$R^T f := \nu \wedge h^f \Big|_{\Gamma\times[0,T]} \tag{1.7}$$

defined on smooth controls vanishing near $t = 0$.

Inverse problem is: *given for a fixed* $T > \operatorname{diam}\Omega$ *operator* R^{2T}*, to recover the manifold* Ω.
The reason of using R^{2T} is the same as in the acoustical case: electromagnetic waves governed by system (1.4)–(1.6), propagate into Ω with velocity 1.

1.3. Nonuiqueness. Setting up the goal to recover Ω, the external observer encounters the following evident obstacle. Let Ω' be such that $\partial\Omega' = \partial\Omega = \Gamma$, and there is a surjective isometry $i : \Omega \to \Omega'$ such that $i|_\Gamma = \mathrm{id}$. Then, for the response operators of systems (1.1)–(1.3) and (1.4)–(1.6) one has ${R'}^T = R^T$ for all $T > 0$. Hence, the map "manifold $\mapsto$ response operator" in not injective. In other words, the observer is not able to distinguish Ω' from Ω via boundary measurements.

So, to determine Ω uniquely is impossible, and we have to clarify the setup of inverse problems. Analyzing the situation, one can recognize that the only reasonable version is:
IP: *given* R^{2T} *for a fixed* $T > \operatorname{diam}\Omega$*, to construct a Riemannian manifold* $\tilde{\Omega}$ *such that* $\partial\tilde{\Omega} = \partial\Omega = \Gamma$ *and* $\tilde{R}^{2T} = R^{2T}$.

Thus, the only thing the observer can hope for, is to construct a *copy* $\tilde{\Omega}$, which responds on the influence of controls in the same way as the original Ω does. Recognizing this fact, a 'philosophical' question arises:
What material can such a copy be constructed from?
The answer, which the rest of the talk is devoted to, is the following:
$\tilde{\Omega}$ is a spectrum of a relevant C*-algebra determined by R^{2T}.

2. Algebras

2.1. Guide. The following is minimal information about algebras: for detail see, e.g., [**9**], [**10**]. By BA and CBA are meant a *Banach* and *commutative Banach algebra* respectively.

(1) A BA is a Banach space $\mathcal{A}$ equipped with the multiplication operation ab satisfying $\|ab\| \le \|a\|\,\|b\|$ $a, b \in \mathcal{A}$. We deal with algebras with the unit $e \in \mathcal{A}$: $ea = ae = a$.

A BA $\mathcal{A}$ is called commutative if $ab = ba$ for all $a, b \in \mathcal{A}$. *Example*: the algebra $C(X)$ of continuous functions with the norm $\|a\| = \sup_X |a(\,\cdot\,)|$

on a topological space X. The subalgebras of $C(X)$ are called function algebras.

A CBA is said to be uniform if $\|a^2\| = \|a\|^2$ holds. All function algebras are uniform.

(2) Let $\mathcal{A}'$ be the dual space. A nonzero functional $\delta \in \mathcal{A}'$ is called a *character* if $\delta(ab) = \delta(a)\delta(b)$. *Example*: a Dirac measure $\delta_{x_0} \in C'(X) : \delta_{x_0}(a) = a(x_0)$ $(x_0 \in X)$. The set of characters endowed with $*$-weak topology (in $\mathcal{A}'$) is called a *spectrum* of $\mathcal{A}$ and denoted by $\widehat{\mathcal{A}}$. Spectrum is a compact Hausdorff space.

(3) The *Gelfand transform* acts from a CBA $\mathcal{A}$ to $C(\widehat{\mathcal{A}})$ by the rule $G\colon a \mapsto \tilde{a}$, $\tilde{a}(\delta) := \delta(a)$, $\delta \in \widehat{\mathcal{A}}$. It represents $\mathcal{A}$ as a function algebra. The passage from $\mathcal{A}$ to $G\mathcal{A} \subset C(\widehat{\mathcal{A}})$ is referred to as *geometrization* of $\mathcal{A}$.

THEOREM 1. *(I.M.Gelfand) If $\mathcal{A}$ is a uniform CBA, then G is an isometric isomorphism from $\mathcal{A}$ onto $G\mathcal{A}$, i.e., $G(\alpha a + \beta b + cd) = \alpha Ga + \beta Gb + Gc\,Gd$ and $\|Ga\|_{C(\widehat{\mathcal{A}})} = \|a\|_{\mathcal{A}}$ holds for all $a, b, c, d \in \mathcal{A}$ and numbers α, β.*

(4) If two CBA $\mathcal{A}$ and $\mathcal{B}$ are isometrically isomorphic (we write $\mathcal{A} \overset{\text{isom}}{=} \mathcal{B}$) via an isometry $j : \mathcal{A} \to \mathcal{B}$, then the dual isometry $j^* : \mathcal{B}' \to \mathcal{A}'$ provides a homeomorphism of their spectra: $j^*\widehat{\mathcal{B}} = \widehat{\mathcal{A}}$. Also, one has $G\mathcal{A} \overset{\text{isom}}{=} G\mathcal{B}$ via the map $G\mathcal{A} \ni Ga \mapsto (Ga) \circ j^* \in G\mathcal{B}$.

(5) If X is a compact Hausdorff space, then the Dirac measures exhaust the spectrum of $C(X)$, whereas the map $i : x_0 \mapsto \delta_{x_0}$ provides a canonical homeomorphism from X onto $\widehat{C(X)}$ (we write $X \overset{\text{hom}}{=} \widehat{C(X)}$). By this, for any $a \in C(X)$ one has $(Ga)(\delta_{x_0}) = a(x_0)$, i.e., Ga is just a pull-back of a via i^{-1}. Thus, algebra $C(X)$ is in fact identical to its Gelfand transform: $GC(X) = C(\widehat{C(X)})$.

(6) Let $\mathcal{I}$ be a norm-closed ideal in a BA $\mathcal{A}$, $\pi : \mathcal{A} \to \mathcal{A}/\mathcal{I}$ the canonical projection "element $\mapsto$ equivalence class". The factor-space $\mathcal{A}/\mathcal{I}$ is endowed with a BA-structure by $\alpha\pi a + \beta\pi b + \pi c\,\pi d := \pi(\alpha a + \beta b + cd)$ and $\|\pi(a)\| := \min\limits_{a' \in \pi(a)} \|a'\|$ for all elements $a, b, c, d \in \mathcal{A}$ and numbers α, β [**9**], [**10**].

(7) For a set $S \subset \mathcal{A}$, by $\vee S$ we denote the minimal norm-closed subalgebra of $\mathcal{A}$, which contains S.

2.2. Algebra $C(\Omega)$. Here we deal with $X = \Omega$, which is our compact Riemannian manifold, and the algebra $C(\Omega)$ of real continuous functions endowed with the standard sup-norm.

Basic facts. We say a set $\sigma \subset \Gamma$ to be *regular* and write $\sigma \in \mathcal{O}_{\text{reg}}(\Gamma)$, if σ is open, connected, and $\partial\sigma$ is smooth. The function

$$d_\sigma(x) := \operatorname{dist}(x, \sigma), \quad x \in \Omega$$

is called a *distance function* with the base σ. Distance functions possess the following well-known geometric properties.

1. They are continuous: $d_\sigma \in C(\Omega)$. For any $x \in \Omega$, there are $\sigma, \sigma' \in \mathcal{O}_{\text{reg}}(\Gamma)$ such that $d_\sigma(x) \neq d_{\sigma'}(x)$, i.e., distance functions distinguish points. No $x \in \Omega$ is their

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mutual zero: $\bigcap_{\sigma\in\mathcal{O}_{\rm reg}(\Gamma)}\{x\in\Omega\,|\,d_\sigma(x)=0\}=\bigcap_{\sigma\in\mathcal{O}_{\rm reg}(\Gamma)}\sigma=\emptyset$. Therefore, by the Stone Theorem [**10**], they generate algebra $C(\Omega)$:

$$\vee\{d_\sigma\,|\,\sigma\in\mathcal{O}_{\rm reg}(\Gamma)\}\,=\,C(\Omega)\,. \tag{2.1}$$

2. Distance functions determine the Riemannian metric on Ω in the following sense. Assume that Ω is given just as a set (without the Riemannian structure), and all d_σ are also known (just as functions on Ω). Then, in Ω one can select the boundary by

$$\Gamma=\{x\in\Omega\,|\,\exists d_\sigma:\ d_\sigma(x)=0\} \tag{2.2}$$

and endow Ω with a differentiable structure by the use of d_σ as local coordinates. Thereafter, in the same distance coordinates, one can recover the metric tensor on Ω [**5**], [**6**].

3. For each $x_0\in\Omega$, a *Dirac measure* $\delta_{x_0}\in C'(\Omega)$, $\delta_{x_0}(a):=a(x_0)$ provides a character of algebra $C(\Omega)$. By 2.1, item 5, $C(\Omega)$ has no another characters and is identical to its Gelfand transform $GC(\Omega)=C(\widehat{C(\Omega)})$.

2.3. Scheme of reconstruction. The trick, which will be used for reconstruction of Ω, is the following. Assume that the external observer possesses the two options:

- from the given R^{2T}, one can determine a 'big' algebra $\mathfrak{B}$, which contains (for the moment, unknown) subalgebra $\mathfrak{C}$ isometric to $C(\Omega)$ via a (for the moment, unknown) isometry $j:C(\Omega)\to\mathfrak{C}\subset\mathfrak{B}$.
- for any regular σ, one can determine the element $jd_\sigma\in\mathfrak{B}$ (also, without the knowledge of j and d_σ!).

In other words, let the observer be able to 'extract' algebra $\mathfrak{B}$ along with the map

$$\mathcal{O}_{\rm reg}(\Gamma)\ni\sigma\overset{\beta}{\mapsto}jd_\sigma\in\mathfrak{B} \tag{2.3}$$

from the inverse data. Then, he can recover the manifold by the following procedure.

Step 1. Determine $\mathfrak{B}$ and β from R^{2T}

Step 2. Construct the subalgebra

$$\mathfrak{C}:=\vee\{\beta\sigma\,|\,\sigma\in\mathcal{O}_{\rm reg}(\Gamma)\}\overset{(2.3)}{=}j\,[\vee\{d_\sigma\,|\,\sigma\in\mathcal{O}_{\rm reg}(\Gamma)\}]\overset{(2.1)}{=}jC(\Omega)\subset\mathfrak{B}\,.$$

Thus, we get an isometric copy $\mathfrak{C}$ of algebra $C(\Omega)$.

Step 3. Find the spectrum $\widehat{\mathcal{C}}$. By construction, we have

$$\widehat{\mathfrak{C}}=(j^*)^{-1}\widehat{C(\Omega)}\overset{\rm hom}{=}\widehat{C(\Omega)}\overset{\rm hom}{=}\Omega$$

(see 2.1, items 4,5). Thus, we get a homeomorphic copy $\tilde\Omega:=\widehat{\mathfrak{C}}$ of the manifold Ω.

However, $\tilde\Omega$ doesn't solve the problem in the full sense of the setup **IP**: one needs to endow it with a Riemannian structure, select the boundary $\tilde\Gamma=\partial\tilde\Omega$, and attach it properly to Γ. So, we continue.

Step 4. Applying the Gelfand transform, construct the algebra $G\mathfrak{C}=C(\tilde\Omega)$. For all regular σ, determine the functions $\tilde d_\sigma:=G\beta\sigma=Gjd_\sigma$ on $\tilde\Omega$.

Thus, we get a set $\tilde\Omega$ (a copy of the original Ω) and functions $\tilde d_\sigma$ (copies of d_σ) on it. As can be checked, in terms of the maps introduced in 2.1, items 4,5, one

has $\tilde{d}_\sigma = d_\sigma \circ i^{-1} \circ j^*$. However, we have succeeded to determine $\tilde{d}_\sigma$ without the knowledge of i, j, and d_σ!

Step 5. By the use of functions $\tilde{d}_\sigma$ as *local coordinates* on $\tilde{\Omega}$, one can recover the differentiable structure on it and determine the distances between points [**6**]. Thus, copy $\tilde{\Omega}$ turns into a Riemannian manifold, which is *isometric* to the original Ω by construction.

Step 6. At last, we need to identify the boundaries of the copy and original. First, define $\tilde{\sigma} := \{\tilde{x} \,|\, \tilde{d}_\sigma(\tilde{x}) = 0\} \subset \tilde{\Omega}$, and determine

$$\tilde{\Gamma} = \{\tilde{x} \in \tilde{\Omega} \,|\, \exists \tilde{d}_\sigma \text{ such that } \tilde{d}_\sigma(\tilde{x}) = 0\} = \bigcup_{\sigma \in \mathcal{O}_{\rm reg}(\Gamma)} \tilde{\sigma} \ \subset \tilde{\Omega}$$

with regard to (2.2). Now, fix an $x \in \Gamma$. Choose $\sigma_1, \sigma_2, ... \in \mathcal{O}_{\rm reg}(\Gamma)$ such that $x = \bigcap\limits_{p \geqslant 1} \sigma_p$. Determine $\tilde{x} = \bigcap\limits_{p \geqslant 1} \tilde{\sigma}_p \in \tilde{\Gamma}$. Then, identify the points by $\Gamma \ni x \equiv \tilde{x} \in \tilde{\Gamma}$.

Thus, the observer gets the Riemannian manifold $\tilde{\Omega}$ such that $\tilde{\Omega} \overset{\rm isom}{=} \Omega$ and $\tilde{\Gamma} \equiv \Gamma$ by construction. As is evident, the inverse data of the copy and original coincide: $\tilde{R}^{2T} = R^{2T}$, so that $\tilde{\Omega}$ solves the **IP**.

In what follows, dealing with concrete cases, it remains for us to determine the relevant algebra $\mathfrak{B}$ and map β from concrete inverse data. Note in advance that each $\mathfrak{B}$ will be a bounded operator algebra on an appropriate Hilbert space.

3. Eikonal algebra in acoustics

3.1. Algebra $\mathfrak{T}$. Reachable sets. Return to the system (1.1)–(1.3). The space of controls $\mathcal{F}^T$ is refereed to as an *outer space* of the system; $\mathcal{H} := L_2(\Omega)$ is its *inner space*. A wave $u^f(\cdot, t) \in \mathcal{H}$ is a *state* of the system (at the moment t).

For a regular σ, define a *reachable set*

$$\mathcal{U}^s_\sigma := \big\{u^f(\,\cdot\,, T) \,|\, \operatorname{supp} f \subset \overline{\sigma} \times [T - s, T]\big\} \ \subset \mathcal{H} \qquad (0 < s \leqslant T) \tag{3.1}$$

initiated by delayed controls acting from σ (here $T - s$ and s mean the value of delay and action time respectively). Denote

- $\Omega^s[\sigma] := \{x \in \Omega \,|\, \operatorname{dist}(x, \sigma) < s\}$ (the metric neighborhood of σ)
- $\mathcal{H}\langle\Omega^s[\sigma]\rangle := \{y \in \mathcal{H} \,|\, \operatorname{supp} y \subset \overline{\Omega^s[\sigma]}\}$ (the subspace of functions supported in $\Omega^s[\sigma]$).

Let a wave u^f be initiated by a control, which acts from σ during s 'seconds' from $t = T - s$ to $t = T$ (so that $u^f(\,\cdot\,, T) \in \mathcal{U}^s_\sigma$ holds). The waves propagate in Ω with the velocity 1. Therefore, $u^f(\cdot, T)$ turns out to be supported in the subdomain $\Omega^s[\sigma]$ only. By the latter, the embedding $\mathcal{U}^s_\sigma \subset \mathcal{H}\langle\Omega^s[\sigma]\rangle$ holds. In the mean time, the fundamental Holmgren-John-Tataru uniqueness theorem provides the density of this embedding:

$$\overline{\mathcal{U}^s_\sigma} \,=\, \mathcal{H}\langle\Omega^s[\sigma]\rangle \qquad (\sigma \in \mathcal{O}_{\rm reg}(\Gamma)) \tag{3.2}$$

(closure in $\mathcal{H}$). So, the waves constitute an L_2-complete system in the domain, which they fill up. This property is referred to as a *local approximate boundary controllability* of the system (1.1)–(1.3). It is the fact, which is a cornerstone of the BC-method: see [**1**]–[**6**].

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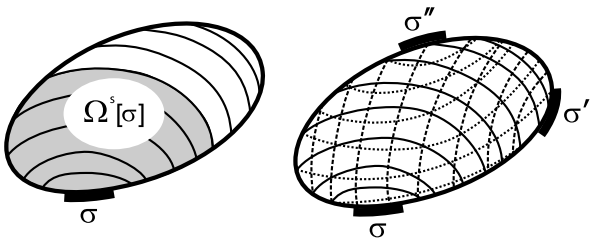

FIGURE 3. Neighborhoods corresponding to eikonals

Projections and eikonals. The (orthogonal) projection P^s_σ in $\mathcal{H}$ onto $\overline{\mathcal{U}^s_\sigma}$ is said to be a *wave projection*. By (3.2), it coincides with the projection onto $\mathcal{H}\langle\Omega^s[\sigma]\rangle$. The latter cuts off functions on $\Omega^s[\sigma]$. As a result, we get the representation

$$P^s_\sigma y \,=\, \begin{cases} y & \text{in } \Omega^s[\sigma] \\ 0 & \text{in } \Omega\backslash\Omega^s[\sigma] \end{cases} . \tag{3.3}$$

Let $0 = s_0 < s_1 < \cdots < s_N = T$ be a partition of $[0,T]$, $\Delta s_i = s_i - s_{i-1}$, $s'_i \in [s_{i-1}, s_i]$, $\Delta P^{s_i}_\sigma = P^{s_i}_\sigma - P^{s_{i-1}}_\sigma$. An operator

$$\tau^T_\sigma \,:=\, \int_0^T s\, dP^s_\sigma = \lim_{\max \Delta s_i \to 0} \sum_{i=1}^N s'_i\, \Delta P^{s_i}_\sigma \tag{3.4}$$

(the convergence in the strong operator topology) is called an *eikonal*. Recall that $d_\sigma(\cdot) := \operatorname{dist}(\cdot, \sigma)$ is a *distance function*. Analyzing the summands in (3.4) with regard to (3.3), one can easily derive

$$(\tau^T_\sigma y)(x) \,=\, \begin{cases} d_\sigma(x)\, y(x), & x \in \Omega^T[\sigma] \\ 0, & x \in \Omega\backslash\Omega^T[\sigma] \end{cases} . \tag{3.5}$$

Note that so simple acting is a consequence of controllability (3.2). Eikonal is a bounded self-adjoint operator in $\mathcal{H}$.

If $T > \operatorname{diam}\Omega$ then $\Omega^T[\sigma] = \Omega$, $P^T_\sigma = \mathbb{I}$, τ^T_σ does not depend on T, and we omit the upper index T. Representation (3.5) takes the form

$$\tau_\sigma\, y \,=\, d_\sigma(\cdot)\, y\,, \tag{3.6}$$

i.e., τ_σ just multiplies by the distance function (that motivates the term 'eikonal').

CONVENTION 1. *In the rest of the paper, we deal with the case* $T > \operatorname{diam}\Omega$.

The algebra. Let $\mathfrak{B}(\mathcal{H})$ be the C*-algebra of bounded operators on $\mathcal{H}$ endowed with the standard operator norm. We have $\tau_\sigma \in \mathfrak{B}(\mathcal{H})$. Define the *eikonal algebra*

$$\mathfrak{T} \,:=\, \vee\{\tau_\sigma \,|\, \sigma \in \mathcal{O}_{\mathrm{reg}}(\Gamma)\} \subset \mathfrak{B}(\mathcal{H})\,.$$

As it follows from (2.1) and (3.6), $\mathfrak{T}$ coincides with the subalgebra of operators multiplying elements of $\mathcal{H}$ by continuous functions. Moreover, the map

$$C(\Omega) \ni \varphi \overset{\alpha}{\mapsto} \check{\varphi} \in \mathfrak{T},$$

where $\check{\varphi}$ is the operator multiplying by φ, is an isometry of algebras since

$$\|\check{\varphi}\|_{\mathfrak{B}(\mathcal{H})} \,=\, \max_\Omega |\varphi(\cdot)| \,=\, \|\varphi\|_{C(\Omega)}$$

holds [**9**], [**10**]. It is the map, which relates the algebra generators:

$$C(\Omega) \ni d_\sigma \overset{\alpha}{\mapsto} \tau_\sigma \in \mathfrak{T}\,. \tag{3.7}$$

3.2. Model. Connecting operator. With the system (1.1)–(1.3) one associates a *connecting operator* $C^T : \mathcal{F}^T \to \mathcal{F}^T$ defined by the relation

$$\big(C^T f, g\big)_{\mathcal{F}^T} = \big(u^f(\,\cdot\,,T), u^g(\,\cdot\,,T)\big)_{\mathcal{H}}\,, \qquad f, g \in \mathcal{F}^T. \tag{3.8}$$

C^T is a positive bounded operator; it connects Hilbert metrics of the outer and inner spaces.

A key fact of the BC-method is that *operator C^T is determined by response operator R^{2T}* via a simple and explicit formula. Namely, one has

$$C^T = 2^{-1}(S^T)^* R^{2T} J^{2T} S^T\,, \tag{3.9}$$

where the map $S^T : \mathcal{F}^T \to \mathcal{F}^{2T}$ extends the controls from $\Gamma \times [0,T]$ to $\Gamma \times [0,2T]$ as odd functions (of time t) with respect to $t = T$; $J^{2T} : \mathcal{F}^{2T} \to \mathcal{F}^{2T}$ is an integration: $(J^{2T} f)(\cdot,t) = \int_0^t f(\cdot,s)\,ds$ (see [**1**], [**3**]).

Models. Recall that Convention 1 is in force.

(1) The subspace
$$\tilde{\mathcal{H}}^T := \overline{[C^T]^{\frac{1}{2}} \mathcal{F}^T} \subset \mathcal{F}^T$$
is said to be a *model interior space* of system (1.1)–(1.3).

(2) For a control $f \in \mathcal{F}^T$, the element
$$\tilde{u}^f(\cdot,T) := [C^T]^{\frac{1}{2}} f \in \tilde{\mathcal{H}}^T$$
is a *model* of the wave $u^f(\cdot,T)$.

(3) The sets
$$\tilde{\mathcal{U}}^s_\sigma := \big\{\tilde{u}^f(\,\cdot\,,T) \,|\, \operatorname{supp} f \subset \overline{\sigma} \times [T-s,T]\big\} \subset \tilde{\mathcal{H}}^T \qquad (0 < s \leqslant T)$$
are the *model reachable sets* (compare with (3.1)).

(4) The projection $\tilde{P}^s_\sigma$ in $\tilde{\mathcal{H}}^T$ onto $\overline{\tilde{\mathcal{U}}^s_\sigma}$ is called a *model wave projection*.

(5) The operator
$$\tilde{\tau}_\sigma := \int_0^T s\, d\, \tilde{P}^s_\sigma \in \mathfrak{B}(\tilde{\mathcal{H}}^T)$$
is a *model eikonal*.

(6) The algebra
$$\tilde{\mathfrak{T}} := \vee\{\tilde{\tau}_\sigma \,|\, \sigma \in \mathcal{O}_{\mathrm{reg}}(\Gamma)\} \subset \mathfrak{B}(\tilde{\mathcal{H}}^T)$$
is a *model* of algebra $\mathfrak{T}$.

Models is the basic notion and ingredient of the BC-method [**1**], [**3**]. There are two reasons of their importance.

- Since
$$\big(\tilde{u}^f(\,\cdot\,,T), \tilde{u}^g(\,\cdot\,,T)\big)_{\tilde{\mathcal{H}}^T} = \Big([C^T]^{\frac{1}{2}} f, [C^T]^{\frac{1}{2}} g\Big)_{\mathcal{F}^T} \overset{(3.8)}{=} \big(u^f(\,\cdot\,,T), u^g(\,\cdot\,,T)\big)_{\mathcal{H}}\,,$$
the map
$$U^T : \mathcal{H} \ni u^f(\,\cdot\,,T) \mapsto \tilde{u}^f(\,\cdot\,,T) \in \tilde{\mathcal{H}}^T$$

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is an isometry[2]. As a consequence, each model mentioned in the list 1.– 6., turns out to be an isometric copy of the corresponding original. In particular, one has $\tilde{P}^s_\sigma := U^T P^s_\sigma (U^T)^*$ that implies

$$\tilde{\tau}_\sigma \;=\; \int_0^T s\, d\, \tilde{P}^s_\sigma = \int_0^T s\, d\, \big[U^T P^s_\sigma (U^T)^*\big] = U^T \tau_\sigma (U^T)^*$$

• Searching the list of models 1.– 6., we see that each of them is eventually determined by the connecting operator C^T. The latter is expressed via R^{2T} by (3.9). Therefore, the models are determined by the inverse data, and, hence, *are accessible for the external observer!*

3.3. Reconstruction. In the viewpoint of the setup **IP**, to recover Ω it remains just to summarize our considerations.

Given R^{2T}, the observer can construct the model algebra $\mathfrak{B}(\tilde{\mathcal{H}}^T)$ and determine the model eikonal $\tilde{\tau}_\sigma$ for any regular σ. In terms of 2.3, the observer gets the algebra $\mathfrak{B} = \mathfrak{B}(\tilde{\mathcal{H}}^T)$ and map $\beta : \sigma \mapsto \tilde{\tau}_\sigma \in \tilde{\mathfrak{T}}$ [3], the model $\tilde{\mathfrak{T}}$ playing the role of the auxiliary algebra $\mathfrak{C}$ in the scheme 2.3.

Then, applying the procedure Step 1 – Step 6, one obtains the copy $\tilde{\Omega}$.

4. Eikonal algebra in electrodynamics

4.1. Maxwell system. Now, consider the system (1.4)–(1.6). The Hilbert space $\vec{L}_2(\Omega)$ of the square-summable vector fields (sections of the tangent bundle $T\Omega$) contains the subspace of curls

$$\mathcal{J} \;:=\; \Big\{ \operatorname{curl} h \;\Big|\; h, \operatorname{curl} h \in \vec{L}_2(\Omega) \Big\}\,,$$

which plays the role of the inner space of the system. Recall that the outer space (of boundary controls) is $\mathcal{F}^T = L_2([0,T]; \vec{L}_2(\Gamma))$.

There is a specific feature of the Maxwell system. In contrast to the acoustic case, its "input→ trajectory" correspondence $\mathcal{F}^T \ni f \mapsto e^f \in L_2\left([0,T]; \mathcal{J}\right)$ is not continuous. Therefore, to be accurate in definitions, we introduce the class

$$\mathcal{F}^T_0 \;:=\; \Big\{ f \in C^\infty([0,T]; \vec{C}^\infty(\Gamma)) \;\Big|\; \operatorname{supp} f \subset (0,T] \Big\}$$

of smooth controls vanishing near $t = 0$. For $f \in \mathcal{F}^T_0$, the solution $\{e^f, h^f\}$ to (1.4)–(1.6) is classical and smooth. The response operator (1.7) is also well defined on $\mathcal{F}^T_0$.

Electric reachable sets. By analogy with (3.1), for a $\sigma \in \mathcal{O}_{\mathrm{reg}}(\Gamma)$, define

$$\mathcal{E}^s_\sigma := \big\{ e^f(\,\cdot\,, T) \,|\, f \in \mathcal{F}^T_0,\, f|_{t<T-s} = 0,\, \operatorname{supp} f(t) \subset \overline{\sigma} \big\} \subset \mathcal{J} \quad (0 < s \leqslant T).$$

Denote $\mathcal{J}\langle \Omega^s[\sigma] \rangle := \{ y \in \mathcal{J} \,|\, \operatorname{supp} y \subset \overline{\Omega^s[\sigma]} \}$. The finiteness of the electromagnetic wave propagation speed in Ω implies $\mathcal{E}^s_\sigma \subset \mathcal{J}\langle \Omega^s[\sigma] \rangle$.

Controllability. The Eller-Isakov-Nakamura-Tataru uniqueness theorem [**8**] leads to the relation

$$\overline{\mathcal{E}^s_\sigma} \;=\; \mathcal{J}\langle \Omega^s[\sigma] \rangle\,, \tag{4.1}$$

[2]Moreover, since $T > \operatorname{diam} \Omega$, the waves $u^f(\cdot, T)$ constitute a complete system in $\mathcal{H}$ (see (3.2)), and U^T turns out to be a *unitary* operator from $\mathcal{H}$ onto $\tilde{\mathcal{H}}^T$.

[3]one has $\tilde{\tau}_\sigma = j d_\sigma$, where $j = \theta \circ \alpha$, α is defined by (3.7), and $\theta : \tau_\sigma \mapsto \tilde{\tau}_\sigma$

which is referred to as a *local boundary controllability* of the Maxwell system. In particular, for $T > \operatorname{diam}\Omega$, one has $\overline{\mathcal{E}^T_\sigma} = \mathcal{J}$.

Projections. Let E^s_σ be the projection in $\mathcal{J}$ onto $\overline{\mathcal{E}^s_\sigma}$. This projection acts in more complicated way than its acoustical analog: its action is not reduced to cutting off fields [4]. Moreover, in the general case, for the different σ and σ' the projections E^s_σ and $E^{s'}_{\sigma'}$ *do not commute*.

Eikonals. Recall that we deal with $T > \operatorname{diam}\Omega$. By (4.1), this implies $\overline{\mathcal{E}^T_\sigma} = \mathcal{J}$ and leads to $E^T_\sigma = \mathbb{I}$ for any σ.

An operator

$$\varepsilon_\sigma := \int_0^T s\, dE^s_\sigma$$

acts in the space $\mathcal{J}$ and is called an *eikonal*. By the aforesaid, it doesn't depend on T and is a bounded positive self-adjoint operator.

In the general case of $\sigma \neq \sigma'$, the eikonals ε_σ and $\varepsilon_{\sigma'}$ do not commute. However, this non-commutativity is weak in the following sense.

THEOREM 2. *(M.N.Demchenko [**6**]) The representation*

$$(\varepsilon_\sigma y)(x) = d_\sigma(x)\, y(x) + \left(K^T y\right)(x), \qquad x \in \Omega \tag{4.2}$$

is valid with a compact operator $K^T : \mathcal{J} \to \vec{L}_2(\Omega)$. By this, for any σ, σ', the commutator $\varepsilon_\sigma \varepsilon_{\sigma'} - \varepsilon_{\sigma'}\varepsilon_\sigma$ is a compact operator in $\mathcal{J}$.

Note that, taken separately, the summands in (4.2) do not belong to the space $\mathcal{J}$.

4.2. Algebra $\dot{\mathfrak{E}}$. Let $\mathfrak{B}(\mathcal{J})$ be the algebra of bounded operators in $\mathcal{J}$. It contains the two-side ideal $\mathfrak{K}(\mathcal{J})$ of compact operators.

Denote by

$$\mathfrak{E} := \vee\{\varepsilon_\sigma \mid \sigma \subset \mathcal{O}_{\mathrm{reg}}(\Gamma)\} \subset \mathfrak{B}(\mathcal{J})$$

the algebra generated by electric eikonals. Also, denote $\mathfrak{K}(\mathfrak{E}) := \mathfrak{E} \cap \mathfrak{K}(\mathcal{J})$ and introduce the factor-algebra

$$\dot{\mathfrak{E}} := \mathfrak{E}/\mathfrak{K}(\mathfrak{E}) = \vee\{\pi\varepsilon_\sigma \mid \sigma \subset \mathcal{O}_{\mathrm{reg}}(\Gamma)\} \subset \mathfrak{B}(\mathcal{J})/\mathfrak{K}(\mathcal{J}),$$

where $\pi : \mathfrak{E} \to \dot{\mathfrak{E}}$ be the canonical "element $\to$ equivalence class" projection.

THEOREM 3. *(M.N.Demchenko [**6**]) Algebra $\dot{\mathfrak{E}}$ is commutative. It is isometrically isomorphic to $C(\Omega)$ via the map, which relates the generators by $C(\Omega) \ni d_\sigma \mapsto \pi\varepsilon_\sigma \in \dot{\mathfrak{E}}$.*

4.3. Solving IP. Connecting operator. A Maxwell *connecting operator* $C^T : \mathcal{F}^T \to \mathcal{F}^T$ is introduced by the relation

$$\left(C^T f, g\right)_{\mathcal{F}^T} = \left(e^f(\,\cdot\,, T), e^g(\,\cdot\,, T)\right)_{\mathcal{J}}, \qquad f, g \in \mathcal{F}^T_0, \tag{4.3}$$

i.e., quite analogously to (3.8). In contrast to the scalar (acoustic) case, it turns out to be an unbounded operator. However, the following principal fact of the BC-method remains valid: operator C^T [5] is determined by the Maxwell response operator R^{2T} via the same relation (3.9) [**3**], [**5**].

[4] see [**3**] for detail

[5] defined on a proper $\operatorname{Dom} C^T \subset \mathcal{F}^T_0$: see [**3**], [**5**]

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Models. The following objects are introduced by perfect analogy with the acoustic case in 3.2.

(1) The subspace $\tilde{\mathcal{J}}^T := \overline{[C^T]^{\frac{1}{2}}\mathcal{F}_0^T} \subset \mathcal{F}^T$ is said to be a *model interior space* of system (1.4)–(1.6).
(2) For a control $f \in \mathcal{F}^T$, the element $\tilde{e}^f(\cdot,T) := [C^T]^{\frac{1}{2}} f \in \tilde{\mathcal{J}}^T$ is a *model* of the electric wave $e^f(\cdot,T)$.
(3) The sets $\tilde{\mathcal{E}}_\sigma^s := \big\{\tilde{e}^f(\,\cdot\,,T) \,|\, \operatorname{supp} f \subset \overline{\sigma} \times [T-s,T]\big\} \subset \tilde{\mathcal{J}}^T \;\; (0 < s \leqslant T)$ are the *model reachable sets*.
(4) The projection $\tilde{E}_\sigma^s$ in $\tilde{\mathcal{J}}^T$ onto $\overline{\tilde{\mathcal{E}}_\sigma^s}$ is called a *model wave projection*.
(5) The operator $\tilde{\varepsilon}_\sigma := \int_0^T s\, d\,\tilde{E}_\sigma^s \in \mathfrak{B}(\tilde{\mathcal{J}}^T)$ is a *model eikonal*.
(6) The algebra $\tilde{\mathfrak{E}} := \vee\{\tilde{\varepsilon}_\sigma \,|\, \sigma \in \mathcal{O}_{\mathrm{reg}}(\Gamma)\} \subset \mathfrak{B}(\tilde{\mathcal{J}}^T)$ is a *model* of algebra $\mathfrak{E}$.
(7) Let $\mathfrak{K}(\tilde{\mathfrak{E}})$ be the ideal of compact operators in $\tilde{\mathfrak{E}}$. The algebra

$$\dot{\tilde{\mathfrak{E}}} := \tilde{\mathfrak{E}}/\mathfrak{K}(\tilde{\mathfrak{E}}) = \vee\{\pi\tilde{\varepsilon}_\sigma \,|\, \sigma \in \mathcal{O}_{\mathrm{reg}}(\Gamma)\} \subset \mathfrak{B}(\tilde{\mathcal{J}}^T)/\mathfrak{K}(\tilde{\mathcal{J}}^T)$$

is a *model* of algebra $\dot{\mathfrak{E}}$. By Demchenko Theorems, there is an isometry $j : C(\Omega) \to \dot{\tilde{\mathfrak{E}}}$, which relates the algebra generators by $j : d_\sigma \mapsto \pi\tilde{\varepsilon}_\sigma$.

Since

$$\big(\tilde{e}^f(\,\cdot\,,T), \tilde{e}^g(\,\cdot\,,T)\big)_{\tilde{\mathcal{J}}^T} = \Big([C^T]^{\frac{1}{2}} f, [C^T]^{\frac{1}{2}} g\Big)_{\mathcal{F}^T} \overset{(4.3)}{=} \big(e^f(\,\cdot\,,T), e^g(\,\cdot\,,T)\big)_{\mathcal{J}} \,,$$

the map

$$U^T : \mathcal{J} \ni e^f(\,\cdot\,,T) \mapsto \tilde{e}^f(\,\cdot\,,T) \in \tilde{\mathcal{J}}^T$$

is an isometry. By this, each model is an isometric copy of the corresponding original. For $T > \operatorname{diam}\Omega$, the waves $e^f(\cdot,T)$ constitute a complete system in $\mathcal{J}$ (see (4.1)), and U^T turns out to be a *unitary* operator from $\mathcal{J}$ onto $\tilde{\mathcal{J}}^T$. By the later, one has $\tilde{E}_\sigma^s = U^T E_\sigma^s (U^T)^*$ that implies

$$\tilde{\varepsilon}_\sigma \,=\, \int_0^T s\, d\,\tilde{E}_\sigma^s = \int_0^T s\, d\,\big[U^T E_\sigma^s (U^T)^*\big] = U^T \varepsilon_\sigma (U^T)^* \,.$$

The crucial fact is the following: as well as in the acoustic case, each model is eventually determined by the connecting operator C^T. The latter is expressed via R^{2T} by (3.9). Therefore, all the models are determined by the inverse data, and are accessible for the external observer.

4.4. Reconstruction. Given the Maxwell response operator R^{2T}, the observer can construct the model algebra $\mathfrak{B}(\tilde{\mathcal{J}}^T)$ and determine the model eikonal $\tilde{\varepsilon}_\sigma$ for any regular σ. Passing to the factor $\mathfrak{B} = \mathfrak{B}(\tilde{\mathcal{J}}^T)/\mathfrak{K}(\tilde{\mathcal{J}}^T)$, the observer determines the generators $\pi\tilde{\varepsilon}_\sigma$ and, hence, gets the map $\beta : \sigma \mapsto \pi\tilde{\varepsilon}_\sigma \in \mathfrak{B}$. By 2.3, it suffices to obtain the copy $\tilde{\Omega}$.

4.5. Comments.

• One of the main ideas of Noncommutative Geometry is that a topological space can be characterized by relevant algebra. In other words, algebras can encode spaces. Our approach follows this idea: inverse data (here, the response operator R^{2T}) determine the eikonal algebra, whereas to recover the space Ω (i.e., to decode information contained in the algebra) is to find the spectrum of this algebra.

• Dealing with the reconstruction problem for a *metric graph* Ω, one can introduce the straightforward analog of the acoustic eikonal algebra $\mathfrak{T}$ [**7**]. However, this analog turns out to be *strongly noncommutative*: no factorization turns $\mathfrak{T}$ into a

commutative algebra. By this, we have to deal with its *Jacobson spectrum* $\widehat{\mathfrak{T}}$, which is the topologized primitive ideal set of $\mathfrak{T}$ [**9**]. General structure of $\mathfrak{T}$ is known [**7**] and related with geometry of Ω but the relation is of rather implicit unclear character. An intriguing fact is that, in some examples, the space $\widehat{\mathfrak{T}}$ is non-Hausdorff. It may contain *clusters*, which are the groups of nonseparable points. Presumably, the clusters of $\widehat{\mathfrak{T}}$ correspond to interior vertices of the graph. Reconstruction $R^{2T} \Rightarrow \Omega$ for graphs is so far an open challenging problem and we hope for our algebraic approach.

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Spectral theory of a mathematical model in quantum field theory for any spin

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Abstract. In this paper we use the formalism of S.Weinberg in order to construct a mathematical model based on the weak decay of hadrons and nuclei. In particular we consider a model which generalizes the weak decay of the nucleus of the cobalt. We associate with this model a Hamiltonian with cutoffs in a Fock space. The Hamiltonian is self-adjoint and has a ground state. By using the commutator theory we get a limiting absorption principle from which we deduce that the spectrum of the Hamiltonian is absolutely continuous above the energy of the ground state and below the first threshold. The coupling constant is supposed sufficiently small and no infrared regularization is assumed.

To my friend James Ralston.

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Acknowledgements
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1. Introduction

This article initiates the study of mathematical models based on the Quantum Field Theory without any restriction concerning the spins of the involved particles.

Precisely, in this paper, we study a mathematical model which generalizes the weak decay of the nucleus ${}^{60}_{27}Co$ of spin 5 into the nucleus ${}^{60}_{28}Ni^*$ of spin 4, one

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electron and the antineutrino associated to the electron. This experiment by C. S. Wu and her collaborators showed that parity conservation is violated in the β decay of atomic nuclei. See [**24**]. The same approach can be applied to many examples of weak decays of hadrons and nuclei with both Fermi and Gamow-Teller transitions. See [**32**] and [**24**].

The mathematical model is based on the construction of free causal fields associated with two massive bosons of spins j_1 and j_2 respectively, a massive fermion of spin j_3 and a massless fermion of helicity $-j_4$ which is the antiparticle of a massless fermion of helicity j_4. These free causal fields are constructed according to the formalism described by S.Weinberg in [**40**–**45**](see also [**36**],[**25**]).

This construction depends on the unitary irreducible representations of the Poincaré group for massive and massless particles and on the finite dimensional representations of $SL(2, \mathbb{C})$ which are both well known. See [**47**], [**46**], [**26**], [**39**], [**37**], [**31**] and [**38**].

The interaction between particles is the one given by S.Weinberg in [**45**, chap 5]. As for the weak interactions we do not suppose that the interaction commutes with space inversion.

After introducing convenient cutoffs for the associated Hamiltonian the mathematical method used to study the spectral properties of the Hamiltonian is based on the one applied to a mathematical model associated with the weak decay of the intermediate vector bosons $W^{\pm}$ into the family of leptons which has been recently developed by [**4**, **10**]. The existence of a ground state and the proof that the spectrum of the Hamiltonian is absolutely continuous above the energy of the ground state and below the first threshold for a sufficiently small coupling constant are our main results. Our methods are largely taken from [**5**, **12**, **17**] and are based on [**2**, **19**, **21**, **23**, **30**, **35**]. No infrared regularization is assumed.

In the framework of non-relativistic QED similar results have been successfully obtained for the massless Pauli-Fierz models (see [**6**–**8**, **11**, **17**, **18**, **20**, **28**] and references therein).

For other mathematical models in Quantum Field Theory see, for example,[**1**, **9**, **13**, **22**] and for string-localized quantum fields see [**33**] and references therein.

The paper is organized as follows.We first recall the free causal fields for massive and massless particles of any spin according to S.Weinberg. We then define the model that we wish to study and prove that the associated Hamiltonian is a self-adjoint operator. We finally prove, for a sufficiently small coupling constant, the existence of a ground state and that the spectrum above the energy of the ground state and below the energy of the first threshold is absolutely continuous. We also determine the full spectrum and give a Limiting Absorption Principle.

2. Free causal fields for massive and massless particles of any spin

In this section we now introduce the free causal fields for massive and massless particles. For that we follow the formalism of S.Weinberg. The construction of quantized fields is mainly based on the Wigner's realizations of the unitary irreducible representations of the Poincaré group. Throughout this work we do not consider space inversion and time reversal transformations because our model describes the weak decay of nuclei which does not conserve the discrete symmetries.

For particles of spin j they are essentially two formalisms: the canonical and the helicity ones. From now on we only consider the helicity formalism because of its

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important usefulness in Physics. From the mathematical point of view there is no difference between the two formalisms. For a description of the unitary irreducible representations of the Poincaré group associated with massive and massless particles see [**46**] and [**27**].

The helicity formalism for massive particles (See [**29**],[**46**] and [**26**]) is associated with the spectral representation of the maximal set of commuting self adjoint operators generated by $(\mathbf{P}, \mathrm{H}^3)$. $\mathbf{P}$ is the generator of space translations and H^3 is the helicity operator $\big(\sqrt{\sum_{i=1}^3 (\mathrm{P}^i)^2}\big)^{-1}(\sum_{l=1}^3 \mathrm{P}^l \mathrm{J}^l)$. The spectrum of H^3 is $(-j, -j+1, \ldots, j-1, j)$.

In the massless case every unitary irreducible representation of the Poincaré group is characterized by its helicity j where $j \in \mathbb{Z}$ or $j \in \mathbb{Z} + \frac{1}{2}$. $|j|$ is then the spin of the particle. From now on we restrict ourselves to the fermionic case. Thus $j \in \mathbb{Z} + \frac{1}{2}$.

The free causal quantized fields associated with massive and massless particles are formal operators defined on the corresponding Fock spaces. They are expressed in terms of the annihilation operators for the particles and of the creation operators for the corresponding antiparticles. In this work we suppose that each particle is distinct from its antiparticle. These quantized fields have to satisfy a relativistic covariance law and a causality condition and they are unique up to an over-all scale. See [**45**, chap 5].

We now introduce Fock spaces and free causal fields.

2.1. Massive particles of any spin.

Consider a particle with mass $m > 0$ and spin j where $j \in \mathbb{N}$ or $j \in \mathbb{N} + \frac{1}{2}$.

Set

$$\mathbb{Z}_j = (-j, -j+1, \ldots, j-1, j) \tag{2.1}$$

and

$$\Sigma_j = \mathbb{R}^3 \times \mathbb{Z}_j \tag{2.2}$$

In the following $(\mathbf{p}, s)$ will be the quantum variables for a massive particle of spin j. Here $\mathbf{p} \in \mathbb{R}^3$ is the momentum and $s \in \mathbb{Z}_j$. In the sequel, we will identify $L^2(\mathbb{R}^3, \mathbb{C}^{2j+1})$ with $L^2(\Sigma_j)$. We shall sometimes use the notations $\xi = (\mathbf{p}, s)$ and $\int_{\Sigma_j} \mathrm{d}\xi = \sum_{s \in \Sigma_j} \int \mathrm{d}^3\mathbf{p}$. The scalar product in $L^2(\Sigma_j)$, $j = 1, 2$ is defined by

$$\big(f, g\big) = \int_{\Sigma_j} \overline{f(\xi)} g(\xi) \mathrm{d}\xi, \quad j = 1, 2.$$

Let $\mathfrak{F}_s^{[m,j]}$ (resp.$\mathfrak{F}_a^{[m,j]}$) be the bosonic (resp. fermionic) Fock space for bosons (resp.fermions) of mass $m > 0$ and spin j. We have

$$\mathfrak{F}_s^{[m,j]} = \bigoplus_{n=0}^{\infty} \otimes_s^n L^2(\Sigma_j). \tag{2.3}$$

where $\otimes_s^n$ denotes the symmetric n-th tensor product and $\otimes_s^0 L^2(\Sigma_j) = \mathbb{C}$.

and

$$\mathfrak{F}_a^{[m,j]} = \bigoplus_{n=0}^{\infty} \otimes_a^n L^2(\Sigma_j). \tag{2.4}$$

where $\otimes_a^n$ denotes the antisymmetric n-th tensor product and $\otimes_a^0 L^2(\Sigma_j) = \mathbb{C}$.

In the case where a massive particle has a distinct antiparticle we introduce a Fock space for both the particle and antiparticle denoted by $\widetilde{\mathfrak{F}}_s^{[m,j]}$ and $\widetilde{\mathfrak{F}}_a^{[m,j]}$ respectively and defined by

$$\begin{aligned}\widetilde{\mathfrak{F}}_s^{[m,j]} &= \mathfrak{F}_s^{[m,j]} \otimes \mathfrak{F}_s^{[m,j]},\\ \widetilde{\mathfrak{F}}_a^{[m,j]} &= \mathfrak{F}_s^{[m,j]} \otimes \mathfrak{F}_a^{[m,j]},\end{aligned} \tag{2.5}$$

We now introduce the creation and annihilation operators for bosons and fermions.

$a_\epsilon(\xi;m,j)$ (resp. $a_\epsilon^*(\xi;m,j)$) is the annihilation (resp.creation) operator for a massive boson of mass $m>0$ and spin j if $\epsilon=+$ and for the corresponding massive antiparticle if $\epsilon=-$.

Similarly, $b_\epsilon(\xi;m,j)$ (resp. $b_\epsilon^*(\xi;m,j)$) is the annihilation (resp.creation) operator for a massive fermion of mass $m>0$ and spin j if $\epsilon=+$ and for the corresponding massive antiparticle if $\epsilon=-$.

See [**34**, section X.7], [**16**, section 4.5], [**10**] and [**14**, section 5.4] for the definition of annihilation and creation operators.

The operators $a_\epsilon(\xi;m,j)$ and $a_\epsilon^*(\xi;m,j)$ fulfill the usual commutation relations (CCR), whereas $b_\epsilon(\xi;m,j)$ and $b_\epsilon^*(\xi;m,j)$ fulfill the canonical anticommutation relation (CAR). See [**45**]. Futhermore, the $a's$ commute with the $b's$.

The following canonical anticommutation and commutation relations hold for a couple of massive particles with $m>0$ and $m'>0$ and spins j and j',

$$\begin{aligned}&\{b_\epsilon(\xi;m,j), b_{\epsilon'}^*(\xi';m',j')\} = \delta_{\epsilon\epsilon'}\delta_{jj'}\delta_{mm'}\delta(\xi-\xi'),\\ &[a_\epsilon(\xi;m,j), a_{\epsilon'}^*(\xi';m',j')] = \delta_{\epsilon\epsilon'}\delta_{jj'}\delta_{mm'}\delta(\xi-\xi'),\\ &\{b_\epsilon(\xi;m,j), b_{\epsilon'}(\xi';m',j')\} = 0,\\ &[a_\epsilon(\xi;m,j), a_{\epsilon'}(\xi';m',j')] = 0,\\ &[b_\epsilon(\xi;m,j), a_{\epsilon'}(\xi';m',j')] = [b_\epsilon(\xi;m,j), a_{\epsilon'}^*(\xi';m',j')] = 0,\end{aligned} \tag{2.6}$$

where $\{b,b'\}=bb'+b'b$ and $[a,a']=aa'-a'a$.

We now introduce

$$\begin{aligned}a_\epsilon(m,j)(\varphi) &= \int_{\Sigma_j} a_\epsilon(\xi;m,j)\overline{\varphi(\xi)}\mathrm{d}\xi,\ a_\epsilon^*(m,j)(\varphi) = \int_{\Sigma_j} a_\epsilon^*(\xi;m,j)\varphi(\xi)\mathrm{d}\xi,\\ b_\epsilon(m,j)(\varphi) &= \int_{\Sigma_j} b_\epsilon(\xi;m,j)\overline{\varphi(\xi)}\mathrm{d}\xi,\ b_\epsilon^*(m,j)(\varphi) = \int_{\Sigma_j} b_\epsilon^*(\xi;m,j)\varphi(\xi)\mathrm{d}\xi.\end{aligned} \tag{2.7}$$

We recall that, for $\varphi\in L^2(\Sigma_j)$, the operators $b_\epsilon(m,j)$ and $b_\epsilon^*(m,j)$ are bounded operators on $\mathfrak{F}_a^{[m,j]}$ satisfying

$$\|b_\epsilon^\sharp(m,j)(\varphi)\| = \|\varphi\|_{L^2}. \tag{2.8}$$

where $b^\sharp$ is b or b^*.

Moreover we have

$$\|a_\epsilon^\sharp(m,j)(N_\epsilon(m,j)+1)^{-\frac{1}{2}}\| \leq \|\varphi\|_{L^2}. \tag{2.9}$$

where $a^\sharp$ is a or a^* and where

$$N_\epsilon(m,j) = \int a_\epsilon^*(\xi;m,j)a_\epsilon(\xi;m,j)d\xi \tag{2.10}$$

Let (J_1,J_2) be two spins such that

$$|J_1-J_2| \leq j \leq J_1+J_2. \tag{2.11}$$

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S.Weinberg has proved the existence of formal causal free fields denoted by

$$\Big(\Psi^{[J_1,J_2]\epsilon}_{M_1M_2}(x)\Big)_{M_1M_2} \tag{2.12}$$

where $M_1 \in (-J_1, -J_1+1, \ldots, J_1-1, J_1)$ and $M_2 \in (-J_2, -J_2+1, \ldots, J_2-1, J_2)$, satisfying a relativistic covariance law and a causality condition. They are unique up to an over-all scale.

See [**44**]and[**27**].

For the helicity formalism we have in the bosonic case

$$\begin{aligned}
&\Psi^{[J_1,J_2]\epsilon}_{M_1M_2}(x)\\
&= (2\pi)^{-3/2}\sum_s \int \mathrm{d}^3\mathbf{p}(u^{[J_1,J_2]}_{M_1M_2})(\mathbf{p},s;m,j)e^{-ip.x}a_\epsilon(\mathbf{p},s;m,j)\\
&+ (2\pi)^{-3/2}\sum_s \int \mathrm{d}^3\mathbf{p}(v^{[J_1,J_2]}_{M_1M_2})(\mathbf{p},s;m,j)e^{ip.x}a^*_{\epsilon'}(\mathbf{p},s;m,j).
\end{aligned} \tag{2.13}$$

where $\epsilon \neq \epsilon'$, with

$$\begin{aligned}
&u^{[J_1,J_2]}_{M_1M_2}(\mathbf{p},s;m,j)\\
&= \frac{1}{\sqrt{2\omega_{\mathbf{p}}}}\sum_{M_1'M_2'} \big(D^{J_1}_{M_1M_1'}(B_{\frac{\mathbf{p}}{|\mathbf{p}|}})D^{J_2}_{M_2M_2'}(B_{\frac{\mathbf{p}}{|\mathbf{p}|}})\\
&\times (\frac{|\mathbf{p}|+\omega_{\mathbf{p}}}{m})^{M_2'-M_1'}(J_1J_2js|J_1M_1'J_2M_2')\big).
\end{aligned} \tag{2.14}$$

and

$$v^{[J_1,J_2]}_{M_1M_2}(\mathbf{p},s;m,j) = (-1)^{j+s}u^{[J_1,J_2]}_{M_1M_2}(\mathbf{p},-s;m,j)\ . \tag{2.15}$$

$D^{J_i}(.)$, $i = 1, 2$, is the unitary irreducible representation of $SU(2)$ defined on a Hilbert space of dimension $2J_i + 1$ that, for simplicity, we suppose to be $\mathbb{C}^{2J_i+1}$. $(J_1J_2js|J_1M_1J_2M_2)$ is the Clebsch-Gordan coefficient in the notation of A.R.Edmonds (see [**15**]) .

$B_{\frac{\mathbf{p}}{|\mathbf{p}|}}$ is an element of $SU(2)$ which is associated with a rotation in $\mathbb{R}^3$ which carries the third axis into the direction of $\mathbf{p}$. We choose

$$B_{\frac{\mathbf{p}}{|\mathbf{p}|}} = \mathrm{e}^{-i\arccos\frac{p^3}{|\mathbf{p}|}(-\frac{p^2}{|\mathbf{p}|}\frac{\sigma_1}{2}+\frac{p^1}{|\mathbf{p}|}\frac{\sigma_2}{2})} \tag{2.16}$$

σ_1 and σ_2 are the two usual 2×2 Pauli matrices.

We have

$$D^J(B_{\frac{\mathbf{p}}{|\mathbf{p}|}}) = \mathrm{e}^{-i\arccos\frac{p^3}{|\mathbf{p}|}(-\frac{p^2}{|\mathbf{p}|}\mathcal{J}_1+\frac{p^1}{|\mathbf{p}|}\mathcal{J}_2)}. \tag{2.17}$$

where $\mathcal{J}_1$ and $\mathcal{J}_2$ are the representations by the standard spin matrices for spin J of the two first generators of the Lie algebra of $SU(2)$.

In the fermionic case the free causal fields are also given by (2.13), (2.14), (2.15), (2.16) and (2.17) after substituting the operators $b_\epsilon(\xi;m,j)$'s for the operators $a_\epsilon(\xi;m,j)$'s.

2.2. Massless fermionic particles of any helicity.

Let $\mathfrak{F}_a^{[j]}$ be the fermionic Fock space for massless fermions of helicity j.

We have

$$\mathfrak{F}_a^{[j]} = \bigotimes_{n=0}^{\infty} \left(\otimes_a^n L^2(\mathbb{R}^3) \right). \tag{2.18}$$

where $\otimes_a^n$ denotes the antisymmetric n-th tensor product and $\otimes_a^0 L^2(\Sigma_j) = \mathbb{C}$.

The operators $b_\epsilon(\mathbf{p}, j)$ and $b_\epsilon^*(\mathbf{p}, j)$ fulfill the canonical anticommutation relation (CAR). See [**45**].

In addition, in the case where several fermions are involved, we follow the convention described in [**45**, sections 4.1 and 4.2]. This means that we will assume that fermionic annihilation and creation operators of different species of particles anticommute (see [**10**, arXiv] for explicit definitions).

Therefore, the following canonical anticommutation relations hold for a couple of massless particles with helicities j and $j' \neq j$ together with a massive particle with $m > 0$ and spin $\widetilde{j}$.

$$\begin{aligned} &\{b_\epsilon(\mathbf{p}, j), b_{\epsilon'}^*(\mathbf{p}', j)\} = \delta_{\epsilon\epsilon'}\delta(\mathbf{p} - \mathbf{p}'), \\ &\{b_\epsilon^\sharp(\mathbf{p}, j), b_{\epsilon'}^\sharp(\mathbf{p}', j')\} = 0, \\ &\{b_\epsilon^\sharp(\xi; m, \widetilde{j}), b_{\epsilon'}^\sharp(\mathbf{p}, j')\} = 0. \end{aligned} \tag{2.19}$$

We now introduce

$$\begin{aligned} b_\epsilon(j)(\varphi) &= \int_{\mathbb{R}^3} b_\epsilon(\mathbf{p}, j)\overline{\varphi(\mathbf{p})}\mathrm{d}^3\mathbf{p}, \\ b_\epsilon^*(j)(\varphi) &= \int_{\mathbb{R}^3} b_\epsilon^*(\mathbf{p}, j)\varphi(\mathbf{p})\mathrm{d}^3\mathbf{p}. \end{aligned} \tag{2.20}$$

For $\varphi \in L^2(\mathbb{R}^3)$, the operators $b_\epsilon(j)$ and $b_\epsilon^*(j)$ are bounded operators on $\mathfrak{F}_a^j$ satisfying

$$\|b_\epsilon^\sharp(j)(\varphi)\| = \|\varphi\|_{L^2}. \tag{2.21}$$

Given two spins J_1 and J_2 S.Weinberg has shown that a unique causal free field for a massless fermion of helicity j associated to the spins J_1 and J_2 can be constructed with the annihilation operator for the massless particle of helicity j and the creation operator for the antiparticle with helicity $-j$ if and only if $j = J_2 - J_1$. The causal field is unique up to an over-all scale.

Thus for every $M_1 \in (-J_1, -J_1 + 1, \ldots, J_1 - 1, J_1)$ and for every $M_2 \in (-J_2, -J_2 + 1, \ldots, J_2 - 1, J_2)$ we denote by $\left(\Phi_{M_1M_2}^{[J_1,J_2]\epsilon}(x)\right)_{M_1M_2}$ the corresponding free causal field.

It follows from [**42**, (3.47)], [**45**, section 5.9] and (2.17) that we have:

$$\begin{aligned} (\Phi_{M_1M_2}^{[J_1,J_2]\epsilon})(x) = (\frac{1}{2\pi})^{\frac{3}{2}} \int \mathrm{d}^3\mathbf{p} \big(&(u_{M_1M_2}^{[J_1,J_2]})(\mathbf{p}, j)\mathrm{e}^{-ip.x} b_\epsilon(\mathbf{p}, j) \\ &+ (v_{M_1M_2}^{[J_1,J_2]})(\mathbf{p}, -j)\mathrm{e}^{ip.x} b_{\epsilon'}^*(\mathbf{p}, -j) \big). \end{aligned} \tag{2.22}$$

where $J_2 - J_1 = j$ and $\epsilon \neq \epsilon'$ with

$$\begin{aligned} &u_{M_1M_2}^{[J_1,J_2]}(\mathbf{p}, j) = v_{M_1M_2}^{[J_1,J_2]}(\mathbf{p}, -j) = (2|\mathbf{p}|)^{J_1+J_2-1/2} \\ &\left(\mathrm{e}^{-i \arccos \frac{p^3}{|\mathbf{p}|}(-\frac{p^2}{|\mathbf{p}|}\mathcal{J}_1^{(1)} + \frac{p^1}{|\mathbf{p}|}\mathcal{J}_2^{(1)})}\right)_{M_1(-J_1)} \left(\mathrm{e}^{-i \arccos \frac{p^3}{|\mathbf{p}|}(-\frac{p^2}{|\mathbf{p}|}\mathcal{J}_1^{(2)} + \frac{p^1}{|\mathbf{p}|}\mathcal{J}_2^{(2)})}\right)_{M_2J_2}. \end{aligned} \tag{2.23}$$

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In addition, in the case where several fermions are involved as for the model we wish to study, we follow the convention described in [**45**, sections 4.1 and 4.2]. This means that we will assume that fermionic annihilation and creation operators of different species of particles anticommute for both massive and massless ones.

3. Definition of the model

We consider a model which is a generalization of the weak decay of the nucleus ${}^{60}_{27}Co$ into the nucleus ${}^{60}_{28}Ni^*$, e^- and $\overline{\nu}_e$.

$$ {}^{60}_{27}Co \rightarrow {}^{60}_{28}\, Ni^* + e^- + \overline{\nu}_e \tag{3.1}$$

$\mathrm{Spin}({}^{60}_{27}Co) = 5$ and $\mathrm{Spin}({}^{60}_{28}Ni^*) = 4$. In this decay parity is not conserved.

Our model involves four particles : two bosons of mass $m_1 > 0$ and spin j_1 and of mass $m_2 > 0$ and spin j_2 respectively, a fermion of mass $m_3 > 0$ and spin j_3 and a massless fermion of helicity $-j_4$ which is the antiparticle of a massless fermion of helicity $j_4 < 0$.

Set $\xi_i = (\mathbf{p}_i, s_i)$ for each $i = 1, 2, 3$, i.e., for the massive bosons and fermion.We have, for each $i = 1, 2, 3$, $\int \mathrm{d}\xi_i = \sum_{s_i} \int \mathrm{d}^3\mathbf{p}_i$.

For the massless fermion we set $\xi_4 = (\mathbf{p}_4, j_4)$ and $\widetilde{\xi_4} = (\mathbf{p}_4, -j_4)$ with $\int \mathrm{d}\xi_4 = \int \mathrm{d}^3\mathbf{p}_4$.

The Fock space of the system is

$$ \mathfrak{F} = \mathfrak{F}_s^{[m_1,j_1]} \otimes \mathfrak{F}_s^{[m_2,j_2]} \otimes \mathfrak{F}_a^{[m_3,j_3]} \otimes \mathfrak{F}_a^{[-j_4]} \tag{3.2}$$

Ω shall denote the vacuum in $\mathfrak{F}$.

The free Hamiltonian H_0 is given by

$$\begin{aligned} H_0 = &\sum_{i=1}^{2} \int w^i(\xi_i) a_+^*(\xi_i; m_i, j_i) a_+(\xi_i; m_i, j_i) \mathrm{d}\xi_i \\ &+ \int w^3(\xi_3) b_+^*(\xi_3; m_3, j_3) b_+(\xi_3; m_3, j_3) \mathrm{d}\xi_3 + \int w^4(\xi_4) b_-^*(\widetilde{\xi_4}) b_-(\widetilde{\xi_4}) \mathrm{d}\xi_4 \end{aligned} \tag{3.3}$$

The free relativistic energies of the massive bosons, the massive fermion and of the massless fermion are given by

$$ w^i(\xi_i) = (|\mathbf{p}_i|^2 + m_i^2)^{1/2}, i = 1, 2, 3 \tag{3.4}$$

$$ w^4(\xi_4) = |\mathbf{p}_4| \tag{3.5}$$

From now on we suppose that

$$\begin{aligned} &m_1 > m_2 > m_3 \\ &m_1 > m_2 + m_3. \end{aligned} \tag{3.6}$$

H_0 is a self-adjoint operator in $\mathfrak{F}$.

In the interaction representation the formal interaction,denoted by $H_I(t)$, is given by

$$ H_I(t) = \int \mathrm{d}^3\mathbf{x} \mathcal{H}(t, \mathbf{x}) \tag{3.7}$$

The S-matrix will be Lorentz-invariant if

$$ \Gamma(U(A, a)) \mathcal{H}(x) \Gamma(U(A, a))^{-1} = \mathcal{H}(\Lambda(A)x + a) \tag{3.8}$$

$$ [\mathcal{H}(x), \mathcal{H}(y)] = 0, (x - y)^2 \leq 0. \tag{3.9}$$

The general form of of $\mathcal{H}(x)$ in terms of the causal free fields is given in [**45**, (5.1.9) and (5.1.10)].

By (2.14) and (2.17) we get for each $i = 1, 2, 3$

$$(u^{[J_1^i,J_2^i]}_{M_1^iM_2^i})(\xi_i; m_i, j_i) = (2\pi)^{-3/2} \tag{3.10}$$
$$\frac{1}{\sqrt{2\omega_{\mathbf{p}_i}}}\Big(\sum_{M_1^{i'}M_2^{i'}} (\frac{|\mathbf{p}_i| + \omega_{\mathbf{p}_i}}{m})^{M_2^{i'}-M_1^{i'}} \big(\mathrm{e}^{-i \arccos \frac{p_i^3}{|\mathbf{p}_i|}(-\frac{p_i^2}{|\mathbf{p}_i|}\mathcal{J}_1^{(i,1)}+\frac{p_i^1}{|\mathbf{p}_i|}\mathcal{J}_2^{(i,1)})}\big)_{M_1^iM_1^{i'}}$$
$$\big(\mathrm{e}^{-i \arccos \frac{p_i^3}{|\mathbf{p}_i|}(-\frac{p_i^2}{|\mathbf{p}_i|}\mathcal{J}_1^{(i,2)}+\frac{p_i^1}{|\mathbf{p}_i|}\mathcal{J}_2^{(i,2)})}\big)_{M_2^iM_2^{i'}} (J_1^iJ_2^ij_is_i|J_1^iM_1^{i'}J_2^iM_2^{i'})\Big).$$

Here $J_\cdot^i$ and $M_\cdot^i$ are associated to the spin of the particle i. $\mathcal{J}_\cdot^{(i,\cdot)}$ are the generators of the rotations in the representation $D^{J_\cdot^i}(\cdot)$.

For the massless fermion by (2.23) we get

$$u^{[J_1^4,J_2^4]}_{M_1^4M_2^4}(\xi_4) = (2|\mathbf{p}_4|)^{J_1^4+J_2^4-1/2}\big(\mathrm{e}^{-i \arccos \frac{p_4^3}{|\mathbf{p}_4|}(-\frac{p_4^2}{|\mathbf{p}_4|}\mathcal{J}_1^{(4,1)}+\frac{p_4^1}{|\mathbf{p}_4|}\mathcal{J}_2^{(4,1)})}\big)_{M_1^4(-J_1^4)} \tag{3.11}$$
$$\big(\mathrm{e}^{-i \arccos \frac{p_2^3}{|\mathbf{p}_2|}(-\frac{p_2^2}{|\mathbf{p}_2|}\mathcal{J}_1^{(4,2)}+\frac{p_4^1}{|\mathbf{p}_4|}\mathcal{J}_2^{(4,2)})}\big)_{M_2^4J_2^4}.$$

where $J_\cdot^4$ and $M_\cdot^4$ are associated to the spin of the massless fermion.

$\mathcal{J}_\cdot^{(4,\cdot)}$ are the generators of the rotations in the representation $D^{J_\cdot^4}(\cdot)$.

We now set for the massive bosons, $i = 1, 2$,

$${}_1\Phi^{[J_1^i,J_2^i]}_{M_1^iM_2^i}(x) = (\frac{1}{2\pi})^{\frac{3}{2}} \int \mathrm{d}\xi_i (u^{[J_1^i,J_2^i]}_{M_1^iM_2^i})(\xi_i; m_i, j_i)\mathrm{e}^{-ip_i.x}a_+(\xi_i; m_i, j_i). \tag{3.12}$$

and for the massive fermion

$${}_1\Psi^{[J_1^3,J_2^3]}_{M_1^3M_2^3}(x) = (\frac{1}{2\pi})^{\frac{3}{2}} \int \mathrm{d}\xi_3 (u^{[J_1^3,J_2^3]}_{M_1^3M_2^3})(\xi_3; m_3, j_3)\mathrm{e}^{-ip_3.x}b_+(\xi_3; m_3, j_3). \tag{3.13}$$

Finally for the massless fermion we let

$$({}_2\Psi^{[J_1^4,J_2^4]}_{M_1^4M_2^4})(x) = (\frac{1}{2\pi})^{\frac{3}{2}} \int \mathrm{d}\xi_4 (u^{[J_1^4,J_2^4]}_{M_1^4M_2^4})(\xi_4)\mathrm{e}^{ip_4.x}b_-^*(\widetilde{\xi_4}). \tag{3.14}$$

Let us now write down the formal interaction,denoted by V_I, of the four particles and antiparticles in the Schrödinger representation.We have

$$V_I = V_I^{(1)} + V_I^{(2)} + \widetilde{V}_I^{(1)} + \widetilde{V}_I^{(2)} \tag{3.15}$$

$V_I^{(1)}$ is given by

$$V_I^{(1)} = \int \mathrm{d}^3\mathbf{x} \sum_{M_1^1M_2^1M_1^2M_2^2M_1^3M_2^3M_1^4M_2^4} \big(g^{(1)}_{M_1^1M_2^1M_1^2M_2^2M_1^3M_2^3M_1^4M_2^4} \tag{3.16}$$
$$\big({}_2\Psi^{[J_1^4,J_2^4]}_{M_1^4M_2^4}\big)(0,\mathbf{x})\big({}_1\Psi^{[J_1^3,J_2^3]}_{M_1^3M_2^3}\big)^*(0,\mathbf{x})\big({}_1\Phi^{[J_1^2,J_2^2]}_{M_1^2M_2^2}\big)^*(0,\mathbf{x})\big({}_1\Phi^{[J_1^1,J_2^1]}_{M_1^1M_2^1}\big)(0,\mathbf{x})\big).$$

$V_I^{(2)}$ is given by

$$V_I^{(2)} = \int \mathrm{d}^3\mathbf{x} \sum_{M_1^1M_2^1M_1^2M_2^2M_1^3M_2^3M_1^4M_2^4} \overline{\big(g^{(1)}_{M_1^1M_2^1M_1^2M_2^2M_1^3M_2^3M_1^4M_2^4}} \tag{3.17}$$
$$\big({}_1\Phi^{[J_1^1,J_2^1]}_{M_1^1M_2^1}\big)^*(0,\mathbf{x})\big({}_1\Phi^{[J_1^2,J_2^2]}_{M_1^2M_2^2}\big)(0,\mathbf{x})\big({}_1\Psi^{[J_1^3,J_2^3]}_{M_1^3M_2^3}\big)(0,\mathbf{x})\big)\big({}_2\Psi^{[J_1^4,J_2^4]}_{M_1^4M_2^4}\big)^*(0,\mathbf{x})\big).$$

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and we have

$$\widetilde{V}_I^{(1)} = \int \mathrm{d}^3\mathbf{x} \sum_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \big(g^{(2)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \big({}_2\Psi^{[J_1^4,J_2^4]}_{M_1^4 M_2^4}\big)(0,\mathbf{x})\big({}_1\Psi^{[J_1^3,J_2^3]}_{M_1^3 M_2^3}\big)^*(0,\mathbf{x})\big({}_1\Phi^{[J_1^2,J_2^2]}_{M_1^2 M_2^2}\big)^*(0,\mathbf{x})\big({}_1\Phi^{[J_1^1,J_2^1]}_{M_1^1 M_2^1}\big)^*(0,\mathbf{x})\big). \tag{3.18}$$

and

$$\widetilde{V}_I^{(2)} = \int \mathrm{d}^3\mathbf{x} \sum_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \big(\overline{g^{(2)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4}} \big({}_1\Phi^{[J_1^1,J_2^1]}_{M_1^1 M_2^1}\big)(0,\mathbf{x})\big({}_1\Phi^{[J_1^2,J_2^2]}_{M_1^2 M_2^2}\big)(0,\mathbf{x})\big({}_1\Psi^{[J_1^3,J_2^3]}_{M_1^3 M_2^3}\big)(0,\mathbf{x})\big)\big({}_2\Psi^{[J_1^4,J_2^4]}_{M_1^4 M_2^4}\big)^*(0,\mathbf{x})\big). \tag{3.19}$$

$\widetilde{V}_I^{(1)}$ and $\widetilde{V}_I^{(2)}$ are responsible for the fact that the bare vacuum will not be an eigenvector of the total Hamiltonian as expected in Physics.

Here A^* is the formal adjoint of A.

V_I is formally self adjoint.

By [**45**, (5.1.10)] the constants $g^{(i)}_{\cdot}$,$i = 1, 2$, have to satisfy the following condition for $i = 1, 2$, and for every $A \in SL(2, \mathbb{C})$

$$g^{(i)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} = \sum_{M_1^{1'} M_2^{1'} M_1^{2'} M_2^{2'} M_1^{3'} M_2^{3'} M_1^{4'} M_2^{4'}} D^{[J_1^1,J_2^1]}_{M_1^{1'} M_2^{1'} M_1^1 M_2^1}(A^{-1}) D^{[J_1^2,J_2^2]}_{M_1^{2'} M_2^{2'} M_1^2 M_2^2}(A^{-1}) D^{[J_1^3,J_2^3]}_{M_1^{3'} M_2^{3'} M_1^3 M_2^3}(A^{-1}) D^{[J_1^4,J_2^4]}_{M_1^{4'} M_2^{4'} M_1^4 M_2^4}(A^{-1}) g^{(i)}_{M_1^{1'} M_2^{1'} M_1^{2'} M_2^{2'} M_1^{3'} M_2^{3'} M_1^{4'} M_2^{4'}}. \tag{3.20}$$

The coefficients $g^{(i)}_{\cdot}$,$i = 1, 2$, are associated with the coupling of the spins J_1^1,J_1^2, J_1^3 and J_1^4 and with the coupling of the spins J_2^1,J_2^2, J_2^3 and J_2^4 to make scalars. See [**45**, section 5],[**40**] and [**44**].

In the Fock space $\mathfrak{F}$ the interaction V_I is a highly singular operator due to the δ-distributions that occur after integrating with respect to $\mathbf{x}$ in the $(V_I^{(\cdot)})'s$ and the $(\widetilde{V}_I^{(\cdot)})'s$ and because of the ultraviolet behavior of the functions $u^{[J_1^{(\cdot)},J_2^{(\cdot)}]}(\cdot)$.

In order to get well defined operators in $\mathfrak{F}$ we have to substitute smoother kernels $F^{(\alpha)}(\xi_1, \xi_2)$, $G^{(\alpha)}(\xi_3)$ and $\widetilde{G}^{(\alpha)}(\xi_4)$, where $\alpha = 1, 2$, for the δ-distributions including the ultraviolet cutoffs.

We then obtain a new operator denoted by H_I and defined as follows in the Schrödinger representation.

$$H_I = H_I^{(1)} + (H_I^{(1)})^* + H_I^{(2)} + (H_I^{(2)})^* \tag{3.21}$$

with

$$gH_I^{(1)} = \tag{3.22}$$
$$(2\pi)^{-3} \sum_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} g^{(1)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \mathrm{d}\xi_4$$
$$F^{(1)}(\xi_1,\xi_2) G^{(1)}(\xi_3) \widetilde{G}^{(1)}(\xi_4)$$
$$\big((u^{[J_1^4,J_2^4]}_{M_1^4 M_2^4})(\xi_4) b^*_-(\widetilde{\xi_4}) \overline{(u^{[J_1^3,J_2^3]}_{M_1^3 M_2^3})(\xi_3;m_3,j_3)} b^*_+(\xi_3;m_3,j_3)\big)\times$$
$$\big(\overline{(u^{[J_1^2,J_2^2]}_{M_1^2 M_2^2})(\xi_2;m_2,j_2)} a^*_+(\xi_2;m_2,j_2) (u^{[J_1^1,J_2^1]}_{M_1^1 M_2^1})(\xi_1;m_1,j_1) a_+(\xi_1;m_1,j_1)\big)\ .$$

and

$$gH_I^{(2)} = \tag{3.23}$$
$$(2\pi)^{-3} \sum_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} g^{(2)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \mathrm{d}\xi_4$$
$$F^{(2)}(\xi_1,\xi_2) G^{(2)}(\xi_3) \widetilde{G}^{(2)}(\xi_4)$$
$$\big((u^{[J_1^4,J_2^4]}_{M_1^4 M_2^4})(\xi_4) b^*_-(\widetilde{\xi_4}) \overline{(u^{[J_1^3,J_2^3]}_{M_1^3 M_2^3})(\xi_3;m_3,j_3)} b^*_+(\xi_3;m_3,j_3)\big)\times$$
$$\big(\overline{(u^{[J_1^2,J_2^2]}_{M_1^2 M_2^2})(\xi_2;m_2,j_2)} a^*_+(\xi_2;m_2,j_2) \overline{(u^{[J_1^1,J_2^1]}_{M_1^1 M_2^1})(\xi_1;m_1,j_1)} a^*_+(\xi_1;m_1,j_1)\big).$$

where

$$g = \sup_\alpha \sup_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} |g^{(\alpha)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4}| \tag{3.24}$$

The total Hamiltonian is then

$$H = H_0 + gH_I \tag{3.25}$$

We now give the conditions that the kernels $F^\alpha(.,.), G^{(\alpha)}(.), \widetilde{G}^{(\alpha)}(.)$ and the coupling constant g have to satisfy in order to associate with the formal operator H a well defined self-adjoint operator in $\mathfrak{F}$.

4. A self-adjoint Hamiltonian

Let $\mathfrak{D}$ denote the set of vectors in $\mathfrak{F}$ for which only a finite number of components are different from zero and each component is smooth with a compact support. See [**10**] for a careful definition. H_0 is essentially self-adjoint on $\mathfrak{D}$. The spectrum of H_0 is $[0,\infty)$ and 0 is a simple eigenvalue with Ω as eigenvector.

The set of thresholds of H_0, denoted by $\mathcal{T}$, is given by

$$\mathcal{T} = \{p\, m_1 + q\, m_2 + r\, m_3; (p,\, q,\, r) \in \mathbb{N}^3 \text{ and } p+q+r \geq 1\}, \tag{4.1}$$

We now need to estimate the functions $(u^{[J_1^i,J_2^i]}_{M_1^i M_2^i})(\xi_i;m_i,j_i)$,where $i = 1,2,3$, and $u^{[J_1^4,J_2^4]}_{M_1^4 M_2^4}(\xi_4)$.

By (2.14) and (2.17) one easily shows that there exist three constants C^i for $i = 1,2,3$ such that

$$|(u^{[J_1^i,J_2^i]}_{M_1^i M_2^i})(\xi_i;m_i,j_i)| \leq C^i \big(1+|\mathbf{p}_i|\big)^{J_1^i+J_2^i-1/2} \tag{4.2}$$

Remark that C^i depends on J_1^i, J_2^i and j_i.

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By (2.23) we obtain

$$|u^{[J_1^4,J_2^4]}_{M_1^4M_2^4}(\xi_4)| \leq (2|\mathbf{p}_4|)^{J_1^4+J_2^4-1/2} \tag{4.3}$$

The estimate (4.3) is verified in the case of neutrinos and antineutrinos of the Standard Model.

From now on the kernels $F^{(\alpha)}(\xi_1,\xi_2)$,$G^{(\alpha)}(\xi_3)$ and $\widetilde{G}^{(\alpha)}(\xi_4)$ are supposed to satisfy the following hypothesis

HYPOTHESIS 4.1. *For $\alpha = 1,2$ we assume*

$$(i) \prod_{\beta=1,2,} \big(1+|\boldsymbol{p}_\beta|\big)^{J_1^\beta+J_2^\beta-1/2} F^{(\alpha)}(.,.) \in L^2(\Sigma_{j_1}\times\Sigma_{j_2})$$

$$(ii)\ \big(1+|\boldsymbol{p}_3|\big)^{J_1^3+J_2^3-1/2} G^{(\alpha)}(.) \in L^2(\Sigma_{j_3})$$

$$(iii)\ |\boldsymbol{p}_4|^{J_1^4+J_2^4-1/2}\widetilde{G}^{(\alpha)}(.) \in L^2(\mathbb{R}^3)$$

REMARK 4.2. Hypothesis 4.1 corresponds to an ultraviolet regularization which breaks the Poincaré invariance of H.

Set

$$\widetilde{F}^{(1)}(\xi_1,\xi_2) = \overline{(u^{[J_1^2,J_2^2]}_{M_1^2M_2^2})(\xi_2;m_2,j_2)}(u^{[J_1^1,J_2^1]}_{M_1^1M_2^1})(\xi_1;m_1,j_1)F^{(1)}(\xi_1,\xi_2). \tag{4.4}$$

$$\widetilde{F}^{(2)}(\xi_1,\xi_2) = \overline{(u^{[J_1^2,J_2^2]}_{M_1^2M_2^2})(\xi_2;m_2,j_2)}\,\overline{(u^{[J_1^1,J_2^1]}_{M_1^1M_2^1})(\xi_1;m_1,j_1))}F^{(2)}(\xi_1,\xi_2). \tag{4.5}$$

For every $\Psi \in \mathfrak{D}$ we have

$$\begin{aligned}\|\int \mathrm{d}\xi_1\mathrm{d}\xi_2(\widetilde{F}^{(1)}(\xi_1,\xi_2))a_+^*(\xi_2;m_2,j_2)a_+(\xi_1;m_1,j_1)\Psi\| \\ \leq C^1C^2\|\big(\prod_{\beta=1,2}(1+|\mathbf{p}_\beta|)^{J_1^\beta+J_2^\beta-1/2}\big)F^{(1)}(.,.)\|_{L^2(\Sigma_{j_1}\times\Sigma_{j_2})} \\ \times\big((\frac{1}{m_1}+\frac{1}{m_2})\|H_0\Psi\|+\frac{1}{2}\|\Psi\|\ \big)\end{aligned} \tag{4.6}$$

$$\begin{aligned}\|\int \mathrm{d}\xi_1\mathrm{d}\xi_2(\widetilde{F}^{(2)}(\xi_1,\xi_2))a_+^*(\xi_2;m_2,j_2)a_+^*(\xi_1;m_1,j_1)\Psi\| \\ \leq C^1C^2\|\big(\prod_{\beta=1,2}(1+|\mathbf{p}_\beta|)^{J_1^\beta+J_2^\beta-1/2}\big)F^{(2)}(.,.)\|_{L^2(\Sigma_{j_1}\times\Sigma_{j_2})} \\ \times\big((\frac{1}{m_1}+\frac{1}{m_2})\|H_0\Psi\|+\|\Psi\|\big)\end{aligned} \tag{4.7}$$

The estimates (4.6) and (4.7) are examples of N_τ estimates.The proof is similar to the one of [**9**, Proposition 3.7] and details are omitted.

Set

$$W(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4) = \Big(|\mathbf{p}_4|^{J_1^4+J^4-1/2}\prod_{\beta=1,2,3}\big(1+|\mathbf{p}_\beta|\big)^{J_1^\beta+J_2^\beta-1/2}\Big) \tag{4.8}$$

$$C_0 = (2\pi)^{-3}C^1C^2C^3\big(\prod_{\beta=1}^{3}(1+2J_1^\beta)^2(1+2J_2^\beta)^2\big)2^{J_1^4+J_2^4-1/2}(1+2J_1^4)(1+2J_2^4) \tag{4.9}$$

and

$$b = \frac{m_1 m_2}{2(m_1+m_2)}. \tag{4.10}$$

We recall that

$$g = \sup_{\alpha} \sup_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} |g^{(\alpha)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4}| \tag{4.11}$$

By (2.8), (2.21), (3.21), (3.22), (3.23), (4.6) and (4.7) we finally get for every $\Psi \in \mathfrak{D}$

$$\begin{aligned} g\|H_I\Psi\| \leq 2gC_0(\frac{1}{m_1}+\frac{1}{m_2})\times \\ \sum_{\alpha=1,2} \|W(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)F^{(\alpha)}(.,.)G^{(\alpha)}(.)\widetilde{G}^{(\alpha)}(.)\|_{L^2(\Sigma_{j_1}\times\Sigma_{j_2}\times\Sigma_{j_3}\times\mathbb{R}^3)} \\ \times (\|H_0\Psi\|+b\|\Psi\|). \end{aligned} \tag{4.12}$$

We then have the following theorem

THEOREM 4.3. *Let $g_1 > 0$ be such that*

$$\begin{aligned} 2C_0 g_1(\frac{1}{m_1}+\frac{1}{m_2}) \sum_{\alpha=1,2} \\ \left(\int \left(W(\boldsymbol{p}_1,\boldsymbol{p}_2,\boldsymbol{p}_3,\boldsymbol{p}_4)\right)^2 \right. \\ \left. |F^{(\alpha)}(\xi_1,\xi_2)|^2 |G^{(\alpha)}(\xi_3)|^2 |\widetilde{G}^{(\alpha)}(\xi_4)|^2 \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3 \mathrm{d}\xi_4 \right)^{1/2} < 1. \end{aligned} \tag{4.13}$$

Then, for every g satisfying $g \leq g_1$, H is a self-adjoint operator in $\mathfrak{F}$ with domain $\mathcal{D}(H_0)$ and $\mathfrak{D}$ is a core for H.

PROOF. By (4.12) the proof of the theorem follows from the Kato-Rellich theorem. □

We now set

$$K(F,G,\widetilde{G}) = \sum_{\alpha=1,2} \|W(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)F^{(\alpha)}(.,.)G^{(\alpha)}(.)\widetilde{G}^{(\alpha)}(.)\|_{L^2(\Sigma_{j_1}\times\Sigma_{j_2}\times\Sigma_{j_3}\times\mathbb{R}^3)}. \tag{4.14}$$

$$C = \frac{C_0}{b}$$

$$B = C_0.$$

By(4.12) we get for every $\Psi \in \mathfrak{D}$

$$\|H_I\Psi\| \leq K(F,G,\widetilde{G})(C\|H_0\Psi\|+B\|\Psi\|) \tag{4.15}$$

5. Main results

We now wish to give two main results. The first one is a statement about the existence of a ground state for the Hamiltonian H together with the location of its spectrum. The second one corresponds to the study of spectrum above the energy of a ground state and below the first threshold

We shall now make the following additional assumptions on the kernels $\widetilde{G}^{(\alpha)}(\xi_4)$.

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HYPOTHESIS 5.1. *There exist constants $K(\widetilde{G})$ and $\widetilde{K}(\widetilde{G})$ such that for $\sigma \geq 0$ and for $\alpha = 1, 2$, $i, l = 1, 2, 3$,*

$$(i) \quad \big(|\boldsymbol{p}_4|^{J_1^4+J_2^4-3/2}\big)\widetilde{G}^{(\alpha)}(\xi_4) \in L^2(\mathbb{R}^3).$$

$$(ii) \quad \left(\int_{|\boldsymbol{p}_4|\leq\sigma} \Big(|\boldsymbol{p}_4|^{2(J_1^4+J_2^4)-1}|\widetilde{G}^{(\alpha)}(\xi_4)|^2 \mathrm{d}\xi_4\right)^{1/2} \leq K(\widetilde{G})\sigma.$$

$$(iii-a) \quad \big(|\boldsymbol{p}_4|^{J_1^4+J_2^4-1/2}\big)\big((\boldsymbol{p}_4\cdot\nabla_{\boldsymbol{p}_4})\widetilde{G}^{(\alpha)}\big)(\xi_4) \in L^2(\mathbb{R}^3).$$

$$(iii-b) \left(\int_{|\boldsymbol{p}_4|\leq\sigma} |\boldsymbol{p}_4|^{2(J_1^4+J_2^4)-1}|\big((\boldsymbol{p}_4\cdot\nabla_{\boldsymbol{p}_4})\widetilde{G}^{(\alpha)}\big)(\xi_4)|^2 \mathrm{d}\xi_4\right)^{1/2} \leq \widetilde{K}(\widetilde{G})\sigma.$$

$$(iii-c) \int_{\mathbb{R}^3} |\boldsymbol{p}_4|^{2(J_1^4+J_2^4)-1}(p_2^i)^2(p_2^l)^2 \left|\frac{\partial^2\widetilde{G}^{(\alpha)}}{\partial p_4^i \partial p_4^l}(\xi_4)\right|^2 \mathrm{d}\xi_4 < \infty.$$

The following theorem is our main first result:

THEOREM 5.2. *Assume that the kernels $F^{(\alpha)}$, $G^{(\alpha)}$ and $\widetilde{G}^{(\alpha)}$, $\alpha = 1, 2$, satisfy Hypothesis 4.1,Hypothesis 5.1(i) and Hypothesis 5.1(ii). Then there exists $g_2 \in (0, g_1]$ such that H has a ground state for $g \leq g_2$. Furthermore, setting*

$$E = \inf \sigma(H)$$

we have

$$\sigma(H) = \sigma_{\mathrm{ess}}(H) = [E, \infty)$$

with $E \leq 0$.

$\sigma_{\mathrm{ess}}(H)$ is the essential spectrum of H.

As in [**10**] and [**4**] our main second result is the proof that the spectrum of H is absolutely continuous in any interval $(\inf\sigma(H), \inf\sigma(H) + m_3 - \delta]$ for $\delta < m_3$ and for g sufficiently small whose smallness depends on δ.

Let p be the operator in $L^2(\mathbb{R}^3)$ accounting for the position of the neutrinos and antineutrinos:

$$p = i\nabla_{\mathbf{p}_2},$$

and set

$$\langle p\rangle = (1 + |p|^2)^{1/2}$$

The second quantized version $\mathrm{d}\Gamma(\langle p\rangle)$ is a self-adjoint operator in $\mathfrak{F}_a(L^2(\mathbb{R}^3)$. We then define the " position" operator P for the antineutrinos in $\mathfrak{F}$ by

$$P = \mathbf{1}\otimes\mathbf{1}\otimes\mathbf{1}\otimes\mathrm{d}\Gamma(\langle p\rangle). \tag{5.1}$$

We then have

THEOREM 5.3. *Suppose that the kernels $F^{(\alpha)}(.,.)$, $G^{(\alpha)}(.)$ and $\widetilde{G}^{(\alpha)}(.)$, $\alpha = 1, 2$, satisfy Hypothesis 4.1 and Hypothesis 5.1. For any $\delta > 0$ satisfying $0 < \delta < m_3$ there exists $g_\delta > 0$ such that for $0 < g \leq g_\delta$:*

(i) *The spectrum of H in $(E, E + m_3 - \delta]$ is absolutely continuous.*
(ii) *For $s > 1/2$, φ and $\psi \in \mathfrak{F}$, the limits*

$$\lim_{\epsilon\to 0}\big(\varphi,\, \langle P\rangle^{-s}(H - \lambda \pm i\epsilon)^{-1}\langle P\rangle^{-s}\psi\big)$$

exist uniformly for λ in every compact subset of $(E, E + m_3 - \delta]$.

(iii) *For* $s \in (1/2,\, 1)$ *the map*

$$\lambda \to \langle P\rangle^{-s}(H - \lambda \pm i0)^{-1}\langle P\rangle^{-s}$$

is locally Hölder continuous of degree $s - 1/2$ *in* $(E, E + m_3 - \delta]$.

(iv) *For* $s \in (1/2,\, 1)$ *and* $f \in C_0^\infty\big((E, E + m_3 - \delta)\big)$ *we have*

$$\|(P+1)^{-s}\mathrm{e}^{-itH}f(H)(P+1)^{-s}\| = \mathcal{O}\big(t^{-(s-1/2)}\big).$$

6. Spectral gap for cutoff operators

In order to prove theorem 5.2 we first need to get an important result about the spectrum of the Hamiltonians with infrared cutoff.

Let us first define the cutoff operators which are the Hamiltonians with infrared cutoff with respect to the momentum of the massless fermion.

For that purpose, let $\chi_0(.) \in C^\infty(\mathbb{R}, [0,1])$ with $\chi_0 = 1$ on $(-\infty, 1]$ and $\chi_0 = 0$ on $[2, \infty]$. For $\sigma > 0$ and $\mathbf{p} \in \mathbb{R}^3$, we set

$$\begin{aligned} &\chi_\sigma(\mathbf{p}) = \chi_0(|\mathbf{p}|/\sigma),\\ &\tilde{\chi}^\sigma(\mathbf{p}) = 1 - \chi_\sigma(\mathbf{p}). \end{aligned} \tag{6.1}$$

The operator $H_{I,\sigma}$ is the interaction given by (3.21), (3.22) and (3.23) associated with the kernel $\tilde{\chi}^\sigma(\mathbf{p}_4)\widetilde{G}^{(\alpha)}(\xi_4)$ instead of $\widetilde{G}^{(\alpha)}(\xi_4)$.

We then set

$$H_\sigma = H_0 + gH_{I,\sigma}. \tag{6.2}$$

We now introduce

$$\begin{aligned} &\Sigma_{4,\sigma} = \mathbb{R}^3 \cap \{|\mathbf{p}_4| < \sigma\}, \qquad \Sigma_4^\sigma = \mathbb{R}^3 \cap \{|\mathbf{p}_4| \geq \sigma\}\\ &\mathfrak{F}_{4,\sigma} = \mathfrak{F}_a(L^2(\Sigma_{4,\sigma})), \qquad\quad \mathfrak{F}_4^\sigma = \mathfrak{F}_a(L^2(\Sigma_4^\sigma)). \end{aligned} \tag{6.3}$$

$\mathfrak{F}_{4,\sigma} \otimes \mathfrak{F}^\sigma$ is the Fock space for the massless fermion.

Now, we set

$$\mathfrak{F}^\sigma = \mathfrak{F}_s^{[m_1,j_1]} \otimes \mathfrak{F}_s^{[m_2,j_2]} \otimes \mathfrak{F}_a^{[m_3,j_3]} \otimes \mathfrak{F}_4^\sigma \text{ and } \quad \mathfrak{F}_\sigma = \mathfrak{F}_{4,\sigma}. \tag{6.4}$$

and we have

$$\mathfrak{F} \simeq \mathfrak{F}^\sigma \otimes \mathfrak{F}_\sigma. \tag{6.5}$$

We further set

$$\begin{aligned} H_0^i &= \int w^i(\xi_i)a_+^*(\xi_i)a_+(\xi_i)\mathrm{d}\xi_i, \quad \text{i=1,2,}\\ H_0^3 &= \int w^3(\xi_3)b_+^*(\xi_3)b_+(\xi_3)\mathrm{d}\xi_3,\\ H_0^4 &= \int w^4(\xi_4)b_-^*(\widetilde{\xi_4})b_-(\widetilde{\xi_4})\mathrm{d}\xi_4. \end{aligned} \tag{6.6}$$

and

$$\begin{aligned} H_0^{4,\sigma} &= \int_{|\mathbf{p}_4|\geq\sigma} w^4(\xi_4)b_-^*(\widetilde{\xi_4})b_-(\widetilde{\xi_4})\mathrm{d}\xi_4,\\ H_{0,\sigma}^4 &= \int_{|\mathbf{p}_4|<\sigma} w^4(\xi_4)b_-^*(\widetilde{\xi_4})b_-(\widetilde{\xi_4})\mathrm{d}\xi_4. \end{aligned} \tag{6.7}$$

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Then, on $\mathfrak{F}^\sigma \otimes \mathfrak{F}_\sigma$, we have

$$H_0^4 = H_0^{4,\sigma} \otimes \mathbf{1}_\sigma + \mathbf{1}^\sigma \otimes H_{0,\sigma}^4, \tag{6.8}$$

where $\mathbf{1}^\sigma$ (resp. $\mathbf{1}_\sigma$) is the identity operator on $\mathfrak{F}^\sigma$ (resp. $\mathfrak{F}_\sigma$).

Using the definitions

$$H^\sigma = H_\sigma|_{\mathfrak{F}^\sigma} \quad \text{and} \quad H_0^\sigma = H_0|_{\mathfrak{F}^\sigma}, \tag{6.9}$$

we get

$$H^\sigma = H_0^1 + H_0^2 + H_0^3 + H_0^{4,\sigma} + gH_{I,\sigma} \quad \text{on } \mathfrak{F}^\sigma, \tag{6.10}$$

and

$$H_\sigma = H^\sigma \otimes \mathbf{1}_\sigma + \mathbf{1}^\sigma \otimes H_{0,\sigma}^4 \quad \text{on } \mathfrak{F}^\sigma \otimes \mathfrak{F}_\sigma. \tag{6.11}$$

Now, for $\delta \in \mathbb{R}$ such that $0 < \delta < m_3$, we define the sequence $(\sigma_n)_{n\geq 0}$ by

$$\begin{aligned} &\sigma_0 = 2m_3 + 1, \\ &\sigma_1 = m_3 - \frac{\delta}{2}, \\ &\sigma_{n+1} = \gamma\sigma_n \text{ for } n \geq 1, \end{aligned} \tag{6.12}$$

where

$$\gamma = 1 - \frac{\delta}{2m_3 - \delta}. \tag{6.13}$$

For $n \geq 0$, we then define the cutoff operators on $\mathfrak{F}^n = \mathfrak{F}^{\sigma_n}$ by

$$H^n = H^{\sigma_n}, \quad H_0^n = H_0^{\sigma_n}, \tag{6.14}$$

and we denote, for $n \geq 0$,

$$E^n = \inf \sigma(H^n). \tag{6.15}$$

We also define the cutoff operators on $\mathfrak{F}$ by

$$H_n = H_{\sigma_n}, \quad H_{0,n} = H_{0,\sigma_n}, \tag{6.16}$$

and we denote, for $n \geq 0$,

$$E_n = \inf \sigma(H_n). \tag{6.17}$$

Note that

$$E^n = E_n \tag{6.18}$$

One easily shows that, for $g \leq g_1$,

$$|E^n| = |E_n| \leq \frac{gK(F, G, \widetilde{G})B}{1 - g_1 K(F, G, \widetilde{G})C} \tag{6.19}$$

See [**4**, **10**] for a proof.

We now set

$$\widetilde{K}(F, G) = \sum_{\alpha=1,2} \| \Big(\prod_{\beta=1,2,3} (1 + |\mathbf{p}_\beta|)^{J_1^\beta + J_2^\beta - 1/2} \Big) F^{(\alpha)}(.,.) G^{(\alpha)}(.) \|_{L^2(\Sigma_{j_1} \times \Sigma_{j_2} \times \Sigma_{j_3})} \, . \tag{6.20}$$

$$\widetilde{C} = \frac{C}{(1 - g_1 K(F, G, \widetilde{G})C)} \tag{6.21}$$

$$\widetilde{B} = \frac{B}{(1 - g_1 K(F,G,\widetilde{G})C)^2} \tag{6.22}$$

$$\widetilde{D}(F,G,\widetilde{G}) \quad = \quad \max\left\{\frac{4(2m_3+1)\gamma}{2m_3-\delta},\ 2\right\}\widetilde{K}(F,G)K(\widetilde{G})\big(2m_3\widetilde{C}\ +\ \widetilde{B}\big)\big) \tag{6.23}$$

Here $K(\widetilde{G})$ is the constant from Hypothesis 5.1(ii).
Let $g_1^{(\delta)}$ be such that

$$0 < g_1^{(\delta)} < \min\left\{1,\ g_1,\ \frac{\gamma-\gamma^2}{3\widetilde{D}(F,G,\widetilde{G})}\right\}\ . \tag{6.24}$$

and let

$$g_3 = \frac{1}{2K(F,G,\widetilde{G})(2C+B)} \tag{6.25}$$

Setting

$$g_2^{(\delta)} = \inf\{g_3, g_1^{\delta)}\} \tag{6.26}$$

and applying the same method as the one used for proving proposition 4.1 in [**4**] we finally get the following result

Proposition 6.1. *Suppose that the kernels $F^{(\alpha)}(.,.)$, $G^{(\alpha)}(.)$ and $\widetilde{G}^{(\alpha)}(.)$, $\alpha = 1,2$, satisfy Hypothesis 4.1 and Hypothesis 5.1(ii). Then, for $g \le g_2^{(\delta)}$, E^n is a simple eigenvalue of H^n for $n \ge 1$, and H^n does not have spectrum in the interval $(E^n,\ E^n + (1 - 3g\frac{\widetilde{D}(F,G,\widetilde{G})}{\gamma})\sigma_n)$.*

7. Proof of theorem 5.2

We adapt the proof of theorem 3.3 in [**10**]. By Proposition 6.1 H^n has a unique ground state, denoted by ϕ^n, in $\mathfrak{F}^n$ such that

$$H^n\phi^n = E^n\phi^n, \quad \phi^n \in \mathcal{D}(H^n), \quad \|\phi^n\| = 1, \quad n \ge 1. \tag{7.1}$$

Therefore H_n has a unique normalized ground state in $\mathfrak{F}$, given by $\tilde{\phi}_n = \phi^n \otimes \Omega_n$, where Ω_n is the vacuum state in $\mathfrak{F}_n$,

$$H_n\tilde{\phi}_n = E^n\tilde{\phi}_n, \quad \tilde{\phi}_n \in \mathcal{D}(H_n), \quad \|\tilde{\phi}_n\| = 1, \quad n \ge 1.$$

Let $H_{I,n}$ be the interaction H_{I,σ_n}. It follows from the pull-through formula that

$$(H_0+H_{I,n})b_-(\widetilde{\xi}_4)\tilde{\phi}_n = E_n b_-(\widetilde{\xi}_4)\tilde{\phi}_n - w^4(\xi_4)b_-(\widetilde{\xi}_4)\tilde{\phi}_n - \big(V_n^1(\xi_4)+V_n^2(\xi_4)\big)\tilde{\phi}_n \tag{7.2}$$

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where

$$V_n^1(\xi_4) = \tag{7.3}$$
$$(2\pi)^{-3} \sum_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} g^{(1)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3$$
$$F^{(1)}(\xi_1,\xi_2) G^{(1)}(\xi_3) \tilde{\chi}^{\sigma_n}(\mathbf{p}_4) \widetilde{G}^{(1)}(\xi_4)$$
$$\Big((u^{[J_1^4,J_2^4]}_{M_1^4 M_2^4})(\xi_4) \overline{(u^{[J_1^3,J_2^3]}_{M_1^3 M_2^3})(\xi_3;m_3,j_3)} b_+^*(\xi_3;m_3,j_3)$$
$$\overline{((u^{[J_1^2,J_2^2]}_{M_1^2 M_2^2})(\xi_2;m_2,j_2)} a_+^*(\xi_2;m_2,j_2) u^{[J_1^1,J_2^1]}_{M_1^1 M_2^1})(\xi_1;m_1,j_1) a_+(\xi_1;m_1,j_1)\Big).$$

and

$$V_n^2(\xi_4) = \tag{7.4}$$
$$(2\pi)^{-3} \sum_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} g^{(2)}_{M_1^1 M_2^1 M_1^2 M_2^2 M_1^3 M_2^3 M_1^4 M_2^4} \int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \mathrm{d}\xi_3$$
$$F^{(2)}(\xi_1,\xi_2) G^{(2)}(\xi_3) \tilde{\chi}^{\sigma_n}(\mathbf{p}_4) \widetilde{G}^{(2)}(\xi_4)$$
$$\Big((u^{[J_1^4,J_2^4]}_{M_1^4 M_2^4})(\xi_4) \overline{(u^{[J_1^3,J_2^3]}_{M_1^3 M_2^3})(\xi_3;m_3,j_3)} b_+^*(\xi_3;m_3,j_3)$$
$$\overline{(u^{[J_1^2,J_2^2]}_{M_1^2 M_2^2})(\xi_2;m_2,j_2)} a_+^*(\xi_2;m_2,j_2) \overline{(u^{[J_1^1,J_2^1]}_{M_1^1 M_2^1})(\xi_1;m_1,j_1)} a_+^*(\xi_1;m_1,j_1)\Big).$$

We obtain

$$\|\big(V_n^1(\xi_4) + V_n^2(\xi_4)\big)\tilde{\phi}_n\| \leq \frac{g}{2} |\mathbf{p}_4|^{J_1^4 + J_2^4 - 1/2} \big(\widetilde{K}(F,G)\big(C\|H_0\tilde{\phi}_n\| + 3B\big). \tag{7.5}$$

It follows from (4.15) that, for every $g \leq g_1$,

$$g\|H_{I,n}\tilde{\phi}_n\| \leq gK(F,G,\widetilde{G})(C\|H_0\tilde{\phi}_n\| + B) \tag{7.6}$$

This yields

$$\|H_0\tilde{\phi}_n\| \leq |E_n| + gK(F,G,\widetilde{G})(C\|H_0\tilde{\phi}_n\| + B) \tag{7.7}$$

By (6.19) and (7.7) we get

$$\|H_0\tilde{\phi}_n\| \leq gK(F,G,\widetilde{G})\big(\frac{1}{(1 - g_1 K(F,G,\widetilde{G})C)^2} + \frac{1}{(1 - g_1 K(F,G,\widetilde{G})C)}\big) \tag{7.8}$$

uniformly with respect to n.

We set

$$M = gK(F,G,\widetilde{G})\big(\frac{1}{(1 - g_1 K(F,G,\widetilde{G})C)^2} + \frac{1}{(1 - g_1 K(F,G,\widetilde{G})C)}\big) \tag{7.9}$$

We then obtain

$$\|b_-(\widetilde{\xi}_4)\tilde{\phi}_n\| \leq gC_0 |\mathbf{p}_4|^{J_1^4 + J_2^4 - 3/2} \big(\sum_{\alpha=1,2} |\widetilde{G}^{(\alpha)}(\xi_4)|\big) \widetilde{K}(F,G)\big((\frac{1}{m_1} + \frac{1}{m_2})M + 3/2\big). \tag{7.10}$$

Thus by Hypothesis 4.1 and Hypothesis 5.1(i) and from (7.10) there exists a constant $\mathcal{O}(F,G,\widetilde{G})>0$ such that

$$\int \|b_-(\widetilde{\xi}_4)\tilde{\phi}_n\|^2 \mathrm{d}\xi_4 \leq g^2\mathcal{O}(F,G,\widetilde{G}) \tag{7.11}$$

uniformly with respect to n.

Since $\|\tilde{\phi}_n\|=1$, there exists a subsequence $(n_k)_{k\geq 1}$, converging to ∞ such that $(\tilde{\phi}_{n_k})_{k\geq 1}$ converges weakly to a state $\tilde{\phi}\in\mathfrak{F}$. By adapting the proof of theorem 4.1 in [**1**,**9**] it follows from (7.11) that there exists g_2 such that $0<g_2\leq g_2^{(\delta)}$ and $\tilde{\phi}\neq 0$ for any $g\leq g_2$. Thus $\tilde{\phi}$ is a ground state of H.

The result about the essential spectrum is obtained by applying the proof given by [**3**] in the case of massless bosons to our model involving massless fermions.For every $\lambda>0$ it is easy to construct a Weyl sequence for H associated with $E+\lambda$. We omit the details.

This concludes the proof of theorem 5.2.

8. Proof of theorem 5.3

The proof of theorem 5.3 depends on the following proposition. A straightforward but lengthy computation shows the following fundamental estimates

PROPOSITION 8.1. *There exists $C(J_1^4,J_2^4)>0$ such that*

$$|p_4^i|\left|\frac{\partial u^{[J_1^4,J_2^4]}_{M_1^4M_2^4}}{\partial p_4^i}(\xi_4)\right| \leq C(J_1^4,J_2^4)|\boldsymbol{p}_4|^{J_1^4+J_2^4-1/2}$$

$$|p_4^i||p_4^l|\left|\frac{\partial^2 u^{[J_1^4,J_2^4]}_{M_1^4M_2^4}}{\partial p_4^i\partial p_4^l}(\xi_4)\right| \leq C(J_1^4,J_2^4)|\boldsymbol{p}_4|^{J_1^4+J_2^4-1/2}$$

for $i,l=1,2,3$.

In the proof of proposition 8.1 we explicitly use the norm of the operators $\mathcal{J}_\cdot^{(2,\cdot)}$ associated with the l^2-norm of $\mathbb{C}^{(2J^2+1)}$.

We now introduce a strict Mourre inequality.

Let us set

$$\tau = 1-\frac{\delta}{2(2m_3-\delta)}\ . \tag{8.1}$$

Let $\chi^{(\tau)}\in C^\infty(\mathbb{R},[0,1])$ be such that

$$\chi^{(\tau)}(\lambda)=\begin{cases} 1 & \text{for } \lambda\in(-\infty,\tau]\,,\\ 0 & \text{for } \lambda\in[1,\infty)\,.\end{cases} \tag{8.2}$$

With the definition (6.12) of $(\sigma_n)_{n\geq 0}$ we set, for all $\mathbf{p}_4\in\mathbb{R}^3$ and $n\geq 1$,

$$\chi_n^{(\tau)}(\mathbf{p}_4)=\chi^{(\tau)}\left(\frac{|\mathbf{p}_4|}{\sigma_n}\right), \tag{8.3}$$

$$a_n^{(\tau)}=\chi_n^{(\tau)}(\mathbf{p}_4)\frac{1}{2}\left(\mathbf{p}_4\cdot i\nabla_{\mathbf{p}_4}+i\nabla_{\mathbf{p}_4}\cdot\mathbf{p}_4\right)\chi_n^{(\tau)}(\mathbf{p}_4), \tag{8.4}$$

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and

$$A_n^{(\tau)} = \mathbf{1} \otimes \mathbf{1} \otimes \mathbf{1} \otimes \mathrm{d}\Gamma(a_n^{(\tau)}) \,, \tag{8.5}$$

The operators $a_n^{(\tau)}$ and $A_n^{(\tau)}$ are self-adjoint and we also have

$$a_n^{(\tau)} = \frac{1}{2} \left(\chi_n^{(\tau)}(\mathbf{p}_4)^2 \mathbf{p}_4 \cdot i\nabla_{\mathbf{p}_4} + i\nabla_{\mathbf{p}_4} \cdot \mathbf{p}_4 \, \chi_n^{(\tau)}(\mathbf{p}_4)^2 \right) . \tag{8.6}$$

Let N *now* be the smallest integer such that

$$N\gamma \geq 1 \ . \tag{8.7}$$

Let us define

$$\epsilon_\gamma = \min \left\{ \frac{1}{2N} \Big(1 - \frac{3g\widetilde{D}(F,G,\widetilde{G})}{\gamma} - \gamma \Big), \, \frac{\tau - \gamma}{4} \right\} \ , \tag{8.8}$$

and choose $f \in C_0^\infty(\mathbb{R})$ such that $0 \leq f \leq 1$ and

$$f(\lambda) = \begin{cases} 1 & \text{if } \lambda \in [(\gamma - \epsilon_\gamma)^2, \, \gamma + \epsilon_\gamma] \,, \\ 0 & \text{if } \lambda > \gamma + 2\epsilon_\gamma \,, \\ 0 & \text{if } \lambda < (\gamma - 2\epsilon_\gamma)^2 \,. \end{cases} \tag{8.9}$$

We now define, for $n \geq 1$,

$$f_n(\lambda) = f\left(\frac{\lambda}{\sigma_n} \right) , \tag{8.10}$$

Let P^n denote the orthogonal projection on the eigenspace corresponding to E^n and let $H_{0,n}^4$ denote H_{0,σ_n}^4.

It follows from Proposition 6.1 that, for $n \geq 1$ and $g \leq g_2^{(\delta)}$,

$$f_n(H_n - E_n) = P^n \otimes f_n(H_{0,n}^4). \tag{8.11}$$

For $E = \inf \sigma(H)$ and any interval Δ, let $E_\Delta(H-E)$ be the spectral projection for the operator $(H-E)$ onto Δ.

Consider, for $n \geq 1$,

$$\Delta_n = [(\gamma - \epsilon_\gamma)^2 \sigma_n, \, (\gamma + \epsilon_\gamma)\sigma_n] \,. \tag{8.12}$$

Now, by adapting the proof of theorem 5.1 (Mourre inequality) in [**4**] and by applying proposition 8.1 together with Hypothesis 4.1 and Hypothesis 5.1(ii), (iii-a) and (iii-b), we prove the existence of a constant $\widetilde{C}_\delta(F,G,\widetilde{G}) > 0$ such that for every $g \leq \inf \left(g_2, g_2^{(\delta)} \right)$ we have

$$f_n(H-E)[H, \, iA_n^{(\tau)}] f_n(H-E) \geq \frac{\gamma^2}{N^2} \sigma_n f_n(H-E)^2 - g\sigma_n \tilde{C}_\delta(F,G,\widetilde{G}). \tag{8.13}$$

Multiplying both sides of (8.13) with $E_{\Delta_n}(H-E)$ we obtain

$$E_{\Delta_n}(H-E)[H, \, iA_n^{(\tau)}] E_{\Delta_n}(H-E) \geq \left(\frac{\gamma^2}{N^2} - g\tilde{C}_\delta(F,G,\widetilde{G}) \right) \sigma_n E_{\Delta_n}(H-E) \,. \tag{8.14}$$

Choosing a constant $g_3^{(\delta)}$ such that

$$g_3^{(\delta)} < \min \left\{ g_2, \, g_2^{(\delta)}, \frac{\gamma^2}{N^2} \frac{1}{\tilde{C}_\delta(F,G,\widetilde{G})} \right\} , \tag{8.15}$$

we finally get the following strict Mourre inequality for every $g \leq g_3^{(\delta)}$ and for $n \geq 1$

$$E_{\Delta_n}(H-E)\,[H,\, iA_n^{(\tau)}]\,E_{\Delta_n}(H-E) \geq C_\delta(F,G,\widetilde{G})\frac{\gamma^2}{N^2}\,\sigma_n\,E_{\Delta_n}(H-E). \tag{8.16}$$

where

$$C_\delta(F,G,\widetilde{G}) = (1 - N^2\tilde{C}_\delta(F,G,\widetilde{G})g_3^{(\delta)}/\gamma^2) > 0. \tag{8.17}$$

After proving a strict Mourre inequality it remains to prove that H is of class $C^2\big(A_n^{(\tau)}\big)$ in order to apply the commutator theory. See [**2**, **19**, **21**, **23**, **30**, **35**].

In fact, according to [**35**], it suffices to prove that H is locally of class $C^2\big(A_n^{(\tau)}\big)$ in $(-\infty, m_3 - \delta/2)$.

This means that, for every $\varphi \in C_0^\infty(-\infty, m_3 - \delta/2)$, $\varphi(H)$ is of class $C^2\big(A_n^{(\tau)}\big)$. Precisely this means that $t \to \mathrm{e}^{-iA_n^{(\tau)}t}\varphi(H)\mathrm{e}^{iA_n^{(\tau)}t}\psi$ is twice continuously differentiable for all $\varphi \in C_0^\infty(-\infty, m_3 - \delta/2)$ and $\psi \in \mathfrak{F}$.

Set

$$A_{n,t}^{(\tau)} = \frac{\mathrm{e}^{-iA_n^{(\tau)}t} - 1}{t} \tag{8.18}$$

By using the proof given in [**10**] H is locally of class $C^2\big(A_n^{(\tau)}\big)$ in $(-\infty, m_3 - \delta/2)$ if we show that

$$\sup_{0<|t|\leq 1} \|[A_{n,t}^{(\tau)},\, [A_{n,t}^{(\tau)},\, H]](H+i)^{-1}\| < \infty \tag{8.19}$$

The operator $a_n^{(\tau)}$ is associated to the following C^∞- vector field in $\mathbb{R}^3$:

$$V_n^{(\tau)}(\mathbf{p}_4) = \chi_n^{(\tau)}(\mathbf{p}_4)^2\mathbf{p}_4 \tag{8.20}$$

Let $\phi_{n,t}^{(\tau)}(.) : \mathbb{R}^3 \to \mathbb{R}^3$ be the corresponding flow generated by $V_n^{(\tau)}(\mathbf{p}_4)$:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\phi_{n,t}^{(\tau)}(\mathbf{p}_4) &= V_n^{(\tau)}\big(\phi_{n,t}(\mathbf{p}_4)\big) \\ \phi_{n,0}^{(\tau)}(\mathbf{p}_4) &= \mathbf{p}_4 \end{aligned} \tag{8.21}$$

We have

$$\mathrm{e}^{-|t|}|\mathbf{p}_4| \leq |\phi_{n,t}^{(\tau)}(\mathbf{p}_4)| \leq \mathrm{e}^{|t|}|\mathbf{p}_4| \tag{8.22}$$

$\phi_{n,t}^{(\tau)}(\mathbf{p}_4)$ induces a one-parameter group of unitary operators $U_n^{(\tau)}(t)$ in $L^2(\mathbb{R}^3)$ defined by

$$\Big(U_n^{(\tau)}(t)f\Big)\,(\mathbf{p}_4) = \Big(\det\nabla\phi_{n,t}^{(\tau)}(\mathbf{p}_4)\Big)^{\frac{1}{2}}\,f(\phi_{n,t}^{(\tau)}(\mathbf{p}_4)). \tag{8.23}$$

$a_n^{(\tau)}$ is the generator of $U_n^{(\tau)}(t)$, i.e.,

$$U_n^{(\tau)}(t) = \mathrm{e}^{-ia_n^{(\tau)}t} \tag{8.24}$$

We have,for every $\psi \in \mathcal{D}(H)$

$$[A_{n,t}^{(\tau)},\, [A_{n,t}^{(\tau)},\, H]]\psi = \frac{1}{t^2}\mathrm{e}^{2iA_n^{(\tau)}t}\left(\mathrm{e}^{-2iA_n^{(\tau)}t}H\mathrm{e}^{2iA_n^{(\tau)}t} - 2\mathrm{e}^{-iA_n^{(\tau)}t}H\mathrm{e}^{iA_n^{(\tau)}t} + H\right)\psi \tag{8.25}$$

In particular we get

$$[A_{n,t}^{(\tau)},\, [A_{n,t}^{(\tau)},\, H_0]]\psi = \frac{1}{t^2}\mathrm{e}^{2iA_n^{(\tau)}t}\left(\mathrm{d}\Gamma(|\phi_{n,2t}^{(\tau)}(\mathbf{p}_4)| - 2|\phi_{n,t}^{(\tau)}(\mathbf{p}_4)| + |\mathbf{p}_4|)\right)\psi. \tag{8.26}$$

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We note that

$$\frac{1}{t^2}\left||\phi^{(\tau)}_{n,2t}(\mathbf{p}_4)|-2|\phi^{(\tau)}_{n,t}(\mathbf{p}_4)|+|\mathbf{p}_4|\right|\leq \sup_{|s|\leq 2|t|}\left|\frac{\partial^2}{\partial s^2}|\phi_{n,s}(\mathbf{p}_4)|\right|, \tag{8.27}$$

Moreover we get

$$\begin{aligned}\frac{\partial^2}{\partial s^2}|\phi_{n,s}(\mathbf{p}_4)| = &-\frac{1}{|\phi_{n,s}(\mathbf{p}_4)|^3}<\phi^{(\tau)}_{n,t}(\mathbf{p}_4, V^{(\tau)}_n(\phi_{n,t}(\mathbf{p}_4))>\\ &+\frac{1}{|\phi_{n,s}(\mathbf{p}_4)|}\|V^{(\tau)}_n(\phi_{n,t}(\mathbf{p}_4))\|^2\\ &+\frac{1}{|\phi_{n,s}(\mathbf{p}_4)|}\Big(<\phi_{n,s}(\mathbf{p}_4), V^{(\tau)}_n(\phi_{n,t}(\mathbf{p}_4))\chi^{(\tau)}_n(\mathbf{p}_4)^2>\\ &+<\frac{\mathbf{p}_4}{|\mathbf{p}_4|}, V^{(\tau)}_n(\phi_{n,t}(\mathbf{p}_4))><\mathbf{p}_4,\phi_{n,t}(\mathbf{p}_4)>\frac{\mathrm{d}}{\mathrm{d}|\mathbf{p}_4|}\chi^{(\tau)}_n(\mathbf{p}_4)^2\Big).\end{aligned} \tag{8.28}$$

where $<.,.>$ is the scalar product in $\mathbb{R}^3$ and $\|.\|$ the corresponding norm.

By (8.22) there exists a constant $c_n>0$ such that

$$\left|\frac{\partial^2}{\partial s^2}|\phi_{n,s}(\mathbf{p}_4)|\right|\leq c_n|\phi^{(\tau)}_{n,t}(\mathbf{p}_4)|\leq c_n\mathrm{e}^{|s|}|\mathbf{p}_4| \tag{8.29}$$

This yields

$$\sup_{0\leq|t|\leq 1}\|[A^{(\tau)}_{n,t},\,[A^{(\tau)}_{n,t},\,H_0]]\,(H_0+1)^{-1}\|\leq c_n\mathrm{e}^2 \tag{8.30}$$

Let

$$\mathcal{G}^{(\alpha)}(\mathbf{p}_4)=u^{[J^4_1,J^4_2]}_{M^4_1M^4_2}(\xi_4)\widetilde{G}^{(\alpha)}(\xi_4) \tag{8.31}$$

and

$$\mathcal{G}^{(\alpha)}_t(\mathbf{p}_4)=\left(\mathrm{e}^{-ia^{(\tau)}_n t}\mathcal{G}^{(\alpha)}\right)(\mathbf{p}_4) \tag{8.32}$$

It follows from (3.21), (3.22) and (3.23) that we can write

$$H_I=\sum_{\alpha=1,2}H_I(F^{(\alpha)},G^{(\alpha)},\mathcal{G}^{(\alpha)}) \tag{8.33}$$

We then have, for every $\psi\in\mathcal{D}(H)$

$$\begin{aligned}[A^{(\tau)}_{n,t},\,[A^{(\tau)}_{n,t},\,H_I]]\psi=&\sum_{\alpha=1,2}\frac{1}{t^2}\mathrm{e}^{2iA^{(\tau)}_n t}\\ &\left(H_I(F^{(\alpha)},G^{(\alpha)},\mathcal{G}^{(\alpha)}_{2t})-2H_I(F^{(\alpha)},G^{(\alpha)},\mathcal{G}^{(\alpha)}_t)+H_I(F^{(\alpha)},G^{(\alpha)},\mathcal{G}^{(\alpha)})\right)\psi\end{aligned} \tag{8.34}$$

By (4.12), (6.20) and (6.22) we get

$$\begin{aligned}\|[A^{(\tau)}_{n,t},\,[A^{(\tau)}_{n,t},\,H_I]]\psi\|\leq &\,g\widetilde{K}(F,G)\\ &\left(\frac{1}{t^2}\sum_{\alpha=1,2}\|\mathcal{G}^{(\alpha)}_{2t}(.)-2\mathcal{G}^{(\alpha)}_t(.)+\mathcal{G}^{(\alpha)}(.)\|_{L^2(\mathbb{R}^3)}\right)^{1/2}(\|H_0\psi\|+b\|\psi\|)\,.\end{aligned} \tag{8.35}$$

Note that, for $0 \leq |t| \leq 1$,

$$\left(\frac{1}{t^2}\sum_{\alpha=1,2}\|\mathcal{G}_{2t}^{(\alpha)}(.) - 2\mathcal{G}_t^{(\alpha)}(.) + \mathcal{G}^{(\alpha)}(.)\|_{L^2(\mathbb{R}^3)}\right)^{1/2} \leq \sup_{0<|s|\leq 2}\Big(\sum_{\alpha=1,2}\Big\|\frac{\partial^2}{\partial s^2}\mathcal{G}_s^{(\alpha)}(.)\Big\|^2_{L^2(\mathbb{R}^3)}\Big)^{1/2}. \tag{8.36}$$

with

$$\begin{aligned}
&\left(\frac{\partial^2}{\partial s^2}(\mathrm{e}^{-ia_n^{(\tau)}s}\mathcal{G}^{(\alpha)})\right)(\mathbf{p}_4)\\
&= \frac{1}{4}\left(\mathrm{e}^{-ia_n^{(\tau)}s}((\mathrm{div}V_n^{(\tau)}(\mathbf{p}_4))^2\mathcal{G}^{(\alpha)})\right)(\mathbf{p}_4)\\
&+ \frac{1}{2}\left(\mathrm{e}^{-ia_n^{(\tau)}s}((\mathrm{div}V_n^{(\tau)}(\mathbf{p}_4))V_n^{(\tau)}(\mathbf{p}_4)\cdot\nabla_{\mathbf{p}_4}\mathcal{G}^{(\alpha)})\right)(\mathbf{p}_4)\\
&+ \frac{1}{2}\left(\mathrm{e}^{-ia_n^{(\tau)}s}(\sum_{i,j=1}^{3}(V_n^{(\tau),i}(\mathbf{p}_4)(\frac{\partial^2}{\partial p_4^i\partial p_4^j}V_n^{(\tau),j}(\mathbf{p}_4)))\mathcal{G}^{(\alpha)})\right)(\mathbf{p}_4)\\
&+ \frac{1}{2}\left(\mathrm{e}^{-ia_n^{(\tau)}s}(\sum_{i,j=1}^{3}V_n^{(\tau),i}(\mathbf{p}_4)\frac{\partial V_n^{(\tau),j}}{\partial p_4^i}(\mathbf{p}_4)\frac{\partial}{\partial p_4^j}\mathcal{G}^{(\alpha)})\right)(\mathbf{p}_4)\\
&+ \frac{1}{2}\left(\mathrm{e}^{-a_n^{(\tau)}s}(\sum_{i,j=1}^{3}V_n^{(\tau),i}(\mathbf{p}_4)V_n^{(\tau),j}(\mathbf{p}_4)\frac{\partial^2}{\partial p_4^i\partial p_4^j}\mathcal{G}^{(\alpha)})\right)(\mathbf{p}_4).
\end{aligned} \tag{8.37}$$

Combining the properties of the C^∞ field $V_n^{(\tau)}(\mathbf{p}_4)$ with Hypothesis 4.1 and 5.1 together with Proposition 8.1 and by mimicking the proof of theorem 5.1 in [**10**] we finally prove (8.19). It follows that H is locally of class $C^2\big(A_n^{(\tau)}\big)$ in $(-\infty, m_3 - \delta/2)$.

By applying the commutator theory (see [**2**, **19**, **21**, **23**, **30**, **35**]) we then get the following Limiting Absorption Principle

THEOREM 8.2. *Suppose that the kernels $F^{(\alpha)}(.,.)$,$G^{(\alpha)}(.)$ and $\widetilde{G}^{(\alpha)}(.)$, $\alpha = 1, 2$, satisfy Hypothesis 4.1 and Hypothesis 5.1. Then, for any $\delta > 0$ satisfying $0 < \delta < m_3$, there exists $g_\delta > 0$ such that, for $0 < g \leq g_\delta$, for $s > 1/2$, φ, $\psi \in \mathfrak{F}$ and for $n \geq 1$, the limits*

$$\lim_{\epsilon\to 0}(\varphi,\, \langle A_n^{(\tau)}\rangle^{-s}(H - \lambda \pm i\epsilon)\langle A_n^{(\tau)}\rangle^{-s}\psi)$$

exist uniformly for $\lambda \in \Delta_n$. Moreover, for $1/2 < s < 1$, the map

$$\lambda \mapsto \langle A_n^{(\tau)}\rangle^{-s}(H - \lambda \pm i0)^{-1}\langle A_n^{(\tau)}\rangle^{-s}$$

is Hölder continuous of degree $s - 1/2$ in Δ_n.

Here $g_\delta = g_3^{(\delta)}$.

Note that there exists a constant $d_n > 0$ such that

$$|a_n^{(\tau)}|^2 \leq d_n\langle b\rangle^2 \tag{8.38}$$

It follows that

$$\left(A_n^{(\tau)}\right)^2 \leq d_n P^2 \tag{8.39}$$

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Now,by adapting the proof of theorem 3.3 in [**4**], we deduce theorem 5.3 from theorem 8.2 and from the following lemma

LEMMA 8.3. *Suppose that* $s \in (1/2, 1)$ *and that for some* n, $f \in C_0^\infty(\Delta_n)$. *Then,*

$$\left\| \langle A_n^{(\tau)} \rangle^{-s} \mathrm{e}^{-itH} f(H) \langle A_n^{(\tau)} \rangle^{-s} \right\| = \mathcal{O}\left(t^{-(s-\frac{1}{2})} \right) .$$

We omit the details.

This concludes the proof of theorem 5.3.

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A review on large k minimal spectral k-partitions and Pleijel's Theorem

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Abstract. In this survey, we review the properties of minimal spectral k-partitions in the two-dimensional case and revisit their connections with Pleijel's Theorem. We focus on the large k problem (and the hexagonal conjecture) in connection with two recent preprints by J. Bourgain and S. Steinerberger on the Pleijel Theorem. This leads us also to discuss some conjecture by I. Polterovich, in relation with square tilings. We also establish a Pleijel Theorem for Aharonov-Bohm Hamiltonians and deduce from it, via the magnetic characterization of the minimal partitions, some lower bound for the number of critical points of a minimal partition.

1. Introduction

We consider the Dirichlet Laplacian in a bounded regular domain $\Omega \subset \mathbb{R}^2$. In [**23**] we have started to analyze the relations between the nodal domains of the real-valued eigenfunctions of this Laplacian and the partitions of Ω by k open sets D_i which are minimal in the sense that the maximum over the D_i's of the ground state energy[1] of the Dirichlet realization of the Laplacian in D_i is minimal. We denote by $\lambda_j(\Omega)$ the increasing sequence of its eigenvalues and by ϕ_j some associated orthonormal basis of real-valued eigenfunctions. The groundstate ϕ_1 can be chosen to be strictly positive in Ω, but the other eigenfunctions ϕ_k must have zerosets. For any real-valued continuous function u on $\overline{\Omega}$, we define the zero set as

$$N(u) = \overline{\{x \in \Omega \mid u(x) = 0\}} \tag{1.1}$$

and call the components of $\Omega \setminus N(u)$ the nodal domains of u. The number of nodal domains of u is called $\mu(u)$. These $\mu(u)$ nodal domains define a k-partition of Ω, with $k = \mu(u)$.

We recall that the Courant nodal Theorem [**16**] (1923) says that, for $k \geq 1$, and if λ_k denotes the k-th eigenvalue of the Dirichlet Laplacian in Ω and $E(\lambda_k)$ the eigenspace associated with λ_k , then, for all real-valued $u \in E(\lambda_k) \setminus \{0\}$, $\mu(u) \leq k$. In dimension 1 the Sturm-Liouville theory says that we have always equality (for Dirichlet in a bounded interval) in the previous theorem (this is what we will call later a Courant-sharp situation). A theorem due to Pleijel [**25**] in 1956 says

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[1]The ground state energy is the smallest eigenvalue.

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that this cannot be true when the dimension (here we consider the $2D$-case) is larger than one. The proof involves lower bounds for the energy of nodal partitions but what is only used is actually that the ground state energy in each of the domain of the partition is the same. This is this link between the proof of Pleijel's Theorem and the lower bounds for the energy of a partition that we would like to explore in this survey, motivated by two recent contributions of J. Bourgain and S. Steinerberger. We will focus on the large k problem (and the hexagonal conjecture). This leads us also to discuss some conjecture by I. Polterovich [**27**], which could be the consequence of a "square" conjecture for some still unknown subclass of partitions. We finally discuss some new consequence of the magnetic characterization of minimal partitions [**21**] for the critical points of this partition.

2. A reminder on minimal spectral partitions

We now introduce for $k \in \mathbb{N}$ ($k \geq 1$), the notion of k-partition. We call **k-partition** of Ω a family $\mathcal{D} = \{D_i\}_{i=1}^k$ of mutually disjoint sets in Ω. We call it **open** if the D_i are open sets of Ω, **connected** if the D_i are connected. We denote by $\mathfrak{O}_k(\Omega)$ the set of open connected partitions of Ω. We now introduce the notion of spectral minimal partition sequence.

Definition 2.1.
For any integer $k \geq 1$, and for $\mathcal{D}$ in $\mathfrak{O}_k(\Omega)$, we introduce

$$\Lambda(\mathcal{D}) = \max_i \lambda(D_i). \tag{2.1}$$

Then we define

$$\mathfrak{L}_k(\Omega) = \inf_{\mathcal{D}\in\mathfrak{O}_k} \Lambda(\mathcal{D}). \tag{2.2}$$

and call $\mathcal{D} \in \mathfrak{O}_k$ a minimal k-partition if $\mathfrak{L}_k = \Lambda(\mathcal{D})$.

More generally we can define, for $p \in [1, +\infty)$, $\Lambda^p(\mathcal{D})$ and $\mathfrak{L}_{k,p}(\Omega)$ by:

$$\Lambda^p(\mathcal{D}) := \left(\frac{\sum \lambda(D_i)^p}{k}\right)^{\frac{1}{p}}, \ \mathfrak{L}_{k,p}(\Omega) = \inf_{\mathcal{D}\in\mathfrak{O}_k} \Lambda^p(\mathcal{D}). \tag{2.3}$$

Note that we can minimize over non necessarily connected partitions and get the connectedness of the minimal partitions as a property (see [**23**]).

If $k = 2$, it is rather well known that $\mathfrak{L}_2 = \lambda_2$ and that the associated minimal 2-partition is a **nodal partition**, i.e. a partition whose elements are the nodal domains of some eigenfunction corresponding to λ_2.

A partition $\mathcal{D} = \{D_i\}_{i=1}^k$ of Ω in $\mathfrak{O}_k$ is called **strong** if

$$\mathrm{Int}\,(\overline{\cup_i D_i}) \setminus \partial\Omega = \Omega\,. \tag{2.4}$$

Attached to a strong partition, we associate a closed set in $\overline{\Omega}$, which is called the **boundary set** of the partition:

$$N(\mathcal{D}) = \overline{\cup_i\,(\partial D_i \cap \Omega)}\,. \tag{2.5}$$

$N(\mathcal{D})$ plays the role of the nodal set (in the case of a nodal partition).

This suggests the following definition of regularity for a partition:

Definition 2.2.
We call a partition $\mathcal{D}$ regular if its associated boundary set $N(\mathcal{D})$, has the following properties:

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(i) Except for finitely many distinct $x_i \in \Omega \cap N$ in the neighborhood of which N is the union of $\nu_i = \nu(x_i)$ smooth curves ($\nu_i \geq 3$) with one end at x_i, N is locally diffeomorphic to a regular curve.
(ii) $\partial\Omega \cap N$ consists of a (possibly empty) finite set of points z_i. Moreover N is near z_i the union of ρ_i distinct smooth half-curves which hit z_i.
(iii) N has the **equal angle meeting property**

The x_i are called the critical points and define the set $X(N)$. A particular role is played by $X^{odd}(N)$ corresponding to the critical points for which ν_i is odd. By **equal angle meeting property**, we mean that the half curves meet with equal angle at each critical point of N and also at the boundary together with the tangent to the boundary.

We say that two elements of the partition D_i, D_j are **neighbors** and write $D_i \sim D_j$, if $D_{ij} := \mathrm{Int}\,(\overline{D_i \cup D_j}) \setminus \partial\Omega$ is connected. We associate with each $\mathcal{D}$ a **graph** $G(\mathcal{D})$ by associating with each D_i a vertex and to each pair $D_i \sim D_j$ an edge. We will say that the graph is **bipartite** if it can be colored by two colors (two neighbors having two different colors). We recall that the graph associated with a collection of nodal domains of an eigenfunction is always bipartite.

REMARK 2.3. *There have been recently very interesting results obtained concerning other kinds of partitions also related to nodal domains. For a generic situation (simple eigenvalues and eigenfunctions without higher order zeros) the nodal domains are in some sense a critical point of a certain functional, see* [**6**]*. In this work there is also an investigation of the nodal deficiency, the difference between k and the number of nodal domains of the k-th eigenfunction. Related results are also obtained in other works about graph Laplacians, partly with the aid of magnetic considerations, see* [**5**]*,* [**4**]*,* [**7**]*. See also* [**15**] *for an elegant approach to the problems considered in* [**4**].

3. Pleijel's Theorem revisited

Pleijel's Theorem as stated in the introduction is the consequence of a more precise theorem and the aim of this section is to present a formalized proof of the historical statement permitting to understand recent improvements and to formulate conjectures.

Generally, the classical proof is going through the proposition

PROPOSITION 3.1.

$$\limsup_{n\to+\infty} \frac{\mu(\phi_n)}{n} \leq \frac{4\pi}{A(\Omega)\liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}}\,. \tag{3.1}$$

Here $\mu(\phi_n)$ is the cardinal of the nodal components of $\Omega \setminus N(\phi_n)$ and $A(\Omega)$ denotes the area of Ω.

Then one establishes a lower bound for $A(\Omega)\liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}$, which should be $> 4\pi$. This property is deduced in [**25**] from the Faber-Krahn inequality which says:

$$(\mathrm{Faber}-\mathrm{Krahn}) \quad A(D)\lambda(D) \geq \lambda(Disk_1)\,, \tag{3.2}$$

for any open set D. Here $Disk_1$ denotes the disk of area 1. Behind the statement of Proposition 3.1, we have actually the stronger proposition:

PROPOSITION 3.2.

$$\limsup_{n\to+\infty} \frac{\mu(\phi_n)}{n} \leq \frac{4\pi}{A(\Omega)\liminf_{k\to+\infty} \frac{L_k(\Omega)}{k}}\,. \tag{3.3}$$

Here $L_k(\Omega)$ denotes the smallest eigenvalue (if any) for which there exists an eigenfunction in $E(L_k)$ with k nodal domains. If no eigenvalue has this property, we simply write $L_k(\Omega) = +\infty$.

The proof of Proposition 3.2 is immediate observing first that for any subsequence n_ℓ, we have

$$\frac{\lambda_{n_\ell}}{n_\ell} \geq \frac{L_{\mu(\phi_{n_\ell})}}{n_\ell} = \frac{L_{\mu(\phi_{n_\ell})}}{\mu(\phi_{n_\ell})} \cdot \frac{\mu(\phi_{n_\ell})}{n_\ell}\,.$$

If we choose the subsequence n_ℓ such that

$$\lim_{\ell\to+\infty} \frac{\mu(\phi_{n_\ell})}{n_\ell} = \limsup_{n\to+\infty} \frac{\mu(\phi_n)}{n}\,,$$

we observe that, by Weyl's formula, we have:

$$N(\lambda) \sim \frac{A(\Omega)}{4\pi}\lambda\,, \tag{3.4}$$

which implies

$$\lim_{\ell\to+\infty} \frac{\lambda_{n_\ell}}{n_\ell} = 4\pi/A(\Omega)\,.$$

We also have

$$\liminf_{\ell\to+\infty} \frac{L_{\mu(\phi_{n_\ell})}}{\mu(\phi_{n_\ell})} \geq \liminf_{k\to+\infty} \frac{L_k(\Omega)}{k}\,.$$

Hence we get the proposition. □

Proposition 3.1 is deduced from Proposition 3.2 by observing that it was established in [**23**] that

$$\lambda_k(\Omega) \leq \mathfrak{L}_k(\Omega) \leq L_k(\Omega)\,. \tag{3.5}$$

The left hand side inequality is a consequence of the variational characterization of λ_k and the right hand side is an immediate consequence of the definitions. Moreover, and this is a much deeper theorem of [**23**], the equalities $\mathfrak{L}_k(\Omega) = L_k(\Omega)$ or $\mathfrak{L}_k(\Omega) = \lambda_k(\Omega)$ imply $\mathfrak{L}_k(\Omega) = L_k(\Omega) = \lambda_k(\Omega)$. We say that, in this case, we are in a Courant sharp situation.

If we think that only nodal partitions are involved in Pleijel's Theorem, it could be natural to introduce $\mathfrak{L}_k^\sharp(\Omega)$ where we take the infimum over a smaller non-empty class of k-partitions $\mathcal{D} = (D_1, \cdots, D_k)$. We call $\mathcal{O}_k^\sharp$ this yet undefined class, which should contain all the nodal k-partitions, if any. Natural candidates for $\mathcal{O}_k^\sharp$ will be discussed in Section 6.

DEFINITION 3.3.

$$\mathfrak{L}_k^\sharp(\Omega) := \inf_{\mathcal{D}\in\mathcal{O}_k^\sharp} \max \lambda(D_i)\,. \tag{3.6}$$

Of course we have always

$$\lambda_k(\Omega) \leq \mathfrak{L}_k(\Omega) \leq \mathfrak{L}_k^\sharp(\Omega) \leq L_k(\Omega)\,. \tag{3.7}$$

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Hence we have:

PROPOSITION 3.4.

$$\limsup_{n\to+\infty} \frac{\mu(\phi_n)}{n} \leq \frac{4\pi}{A(\Omega)\liminf_{k\to+\infty} \frac{\mathfrak{L}_k^\sharp(\Omega)}{k}}\,, \tag{3.8}$$

Hence this is the right hand side of (3.8) which seems to be interesting to analyze.

It is clear from (3.7) that all these upper bounds are less than one, which corresponds to a weak asymptotic version of Courant's Theorem.

We now come back to the proof by Pleijel of his theorem. We apply the Faber-Krahn inequality (3.2) to any element D_i of the minimal k-partition $\mathcal{D}$, and summing up, we immediately get:

$$A(\Omega)\frac{\mathfrak{L}_k(\Omega)}{k} \geq \lambda(Disk_1)\,. \tag{3.9}$$

Implementing this inequality in Proposition 3.2, we immediately get:

THEOREM 3.5 (Pleijel).

$$\limsup_{n\to+\infty} \frac{\mu(\phi_n)}{n} \leq \nu_{Pl}\,, \tag{3.10}$$

with

$$\nu_{Pl} = \frac{4\pi}{\lambda(Disk_1)} \sim 0.691\,.$$

REMARKS 3.6.

(i) *We note that the proof of Pleijel uses only a weak form of* (3.9)*, where* $\mathfrak{L}_k$ *is replaced by* L_k*.*

(ii) *Note that the same result is true in the Neumann case (Polterovich* [**27**]*) under some analyticity assumption on the boundary. Note also that computations for the square were already presented in* [**25**]*.*

(iii) *Note that we have the better:*

$$A(\Omega)\frac{\mathfrak{L}_{k,1}(\Omega)}{k} \geq \lambda(Disk_1)\,. \tag{3.11}$$

But this improvement has no effect on Pleijel's Theorem. In particular, we recall that we do not have necessarily $\lambda_k(\Omega) \leq \mathfrak{L}_{k,1}(\Omega)$ *(take* $k = 2$ *and use the criterion of Helffer–Hoffmann-Ostenhof* [**19**]*). This inequality can be replaced (see* [**19**]*) by:*

$$\mathfrak{L}_{k,1}(\Omega) \geq \frac{1}{k}\sum_{\ell=1}^{k} \lambda_\ell(\Omega)\,. \tag{3.12}$$

Again a Weyl asymptotic shows that this last inequality is strict for k *large. We have indeed as* $k \to +\infty$

$$\frac{1}{k}\sum_{\ell=1}^{k} \lambda_\ell(\Omega) \sim \frac{2\pi k}{A(\Omega)}\,,$$

to compare with (3.11)*.*

(iv) *Pleijel's Theorem is valid in the case of the Laplace-Beltrami operator on a compact manifold (see some survey inside* [**3**] *or* [**2**]*).*

Around the hexagonal conjecture.
It is rather easy (see [**12**]) using hexagonal tilings to prove that:

$$A(\Omega)\liminf_{k\to+\infty}\frac{\mathfrak{L}_k(\Omega)}{k}\leq A(\Omega)\limsup_{k\to+\infty}\frac{\mathfrak{L}_k(\Omega)}{k}\leq\lambda(Hexa_1)\,, \tag{3.13}$$

where $Hexa_1$ is the regular hexagon of area 1.

Note that any tiling leads to a similar upper bound but $\lambda(Hexa_1)$ gives to our knowledge the smallest lower bound for a fundamental cell of area 1. Here are a few numerical (sometimes exact) values corresponding to the $Hexa_1$, T_1, and Sq_1 being respectively a regular hexagon, a square of area 1 and an equilateral triangle:

$$\lambda_1(Hexa_1)\sim 18.5901\ ,\ \lambda_1(Sq_1)=2\pi^2\sim 19.7392\ ,\ \lambda_1(T_1)\sim 22.7929\,. \tag{3.14}$$

In addition it is not known that the regular hexagon with area 1 has the lowest groundstate eigenvalue among all hexagons of the same area. (famous conjecture of Polya and Szegö).

A now well known conjecture (hexagonal conjecture) (Van den Berg, Caffarelli-Lin [**14**]) was discussed in Helffer–Hoffmann-Ostenhof–Terracini [**23**], Bonnaillie-Helffer-Vial [**12**], Bourdin-Bucur-Oudet [**10**] and reads as follows:

Conjecture 3.7.

$$A(\Omega)\liminf_{k\to+\infty}\frac{\mathfrak{L}_k(\Omega)}{k}=A(\Omega)\limsup_{k\to+\infty}\frac{\mathfrak{L}_k(\Omega)}{k}=\lambda(Hexa_1) \tag{3.15}$$

The minimal partitions corresponding to $\mathfrak{L}_{k,1}$ were computed for the torus by Bourdin-Bucur-Oudet [**10**]. This conjecture would lead to the conjecture that in Pleijel's estimate we have actually:

Conjecture 3.8. *(Hexagonal conjecture for Pleijel)*

$$A(\Omega)\limsup_{n\to+\infty}\frac{\mu(\phi_n)}{n}\leq\nu_{Hex}\,, \tag{3.16}$$

with

$$\nu_{Hex}=\frac{4\pi}{\lambda(Hexa_1)}\sim 0.677\,.$$

We note indeed that

$$\frac{\nu_{Hex}}{\nu_{Pl}}=\frac{\lambda(Disk_1)}{\lambda(Hexa_1)}\sim 0.977\,.$$

We now come back to the enigmatic Proposition 3.4 and consider the asymptotic behavior of $\frac{\mathfrak{L}_k^\sharp(\Omega)}{k}$ as $k\to+\infty$. A first indication that our choice of $\Omega^\#$ is promising would be to show that the following property holds.

Property 3.9.

$$A(\Omega)\liminf_{k\to+\infty}\frac{\mathfrak{L}_k^\sharp(\Omega)}{k}\geq\lambda(Sq_1)\,. \tag{3.17}$$

where Sq_1 denotes the unit square.

The proof of this property should mimic what was done for $\mathfrak{L}_k(\Omega)$ (see for example [**12**] or [**14**]), but replacing hexagonal tilings by square tilings.

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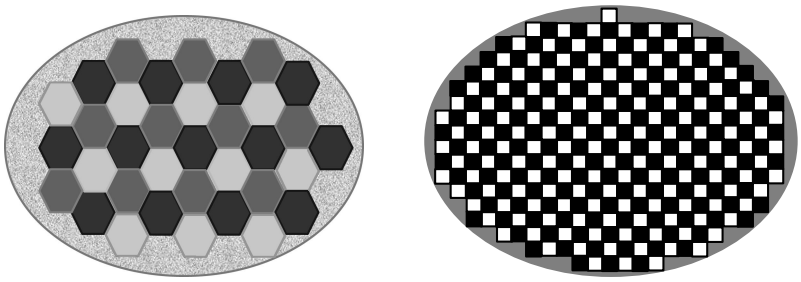

FIGURE 1. Non exhaustive hexagonal or square tilings inside an open set Ω

The philosophy behind the choice of $\Omega_k^\sharp$ should be the following: the hexagonal conjecture for k-partitions should be replaced by the square conjecture when bipartite k-partitions are involved because square tilings can be colored by two colors with the rule that two neighbors have two different colors.

Note that the existence of classes $\mathcal{O}_k^\sharp$ ($k \in \mathbb{N}^*$) such that Property 3.9 is satisfied would give a proof of the conjecture:

CONJECTURE 3.10. *(Polterovich)*

$$\limsup_{n\to+\infty} \frac{\mu(\phi_n)}{n} \leq \frac{4\pi}{\lambda(Sq_1)} = \frac{2}{\pi}\,. \tag{3.18}$$

This conjecture is due to Iosif Polterovich [**27**] on the basis of computations for the rectangle of Blum-Gutzman-Smilansky [**9**]. Due to the computations on the square [**25**] (see however the discussion in Section 5), together with computations for the rectangle [**28**], this should be the optimal result.

4. Improving the use of the Faber-Krahn Inequality

4.1. Preliminaries. This section is devoted to reporting on the two previously mentioned results by J. Bourgain and S. Steinerberger. Although not explicitly written in this way, the goal of Bourgain [**11**] and Steinerberger [**29**] was to improve Pleijel's proof by improving the lower bound of $\liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}$. Bourgain gives a rough estimate of his improvement with a size of 10^{-9}.

In any case, it is clear from their proof that this will lead to a statement where in (3.10) ν_{Pl} is replaced by

$$\nu_{Hex} \leq \nu_{Bo} < \nu_{Pl}\,,$$

and

$$\nu_{Hex} \leq \nu_{St} < \nu_{Pl}\,,$$

where ν_{Bo} and ν_{St} are the constants obtained respectively by Bourgain and Steinerberger.

4.2. Bourgain's improvement [**11**]**.** One ingredient is a refinement of the Faber-Krahn inequality du to Hansen-Nadirashvili [**18**]:

LEMMA 4.1 (Hansen-Nadirashvili).
For a nonempty simply connected bounded domain $\Omega \subset \mathbb{R}^2$, we have

$$A(\Omega)\,\lambda(\Omega) \geq \left(1 + \frac{1}{250}(1 - \frac{r_i(\Omega)}{r_0(\Omega)})^2\right) \lambda(\mathrm{Disk}_1)\,, \tag{4.1}$$

with $r_0(\Omega)$ the radius of the disk of same area as Ω and $r_i(\Omega)$ the inradius of Ω.

Actually, J. Bourgain needs (and gives) an additional argument for treating non simply connected domains. In the right hand side of (4.1) not only the inradius occurs but also the smallest area of the components of $\mathbb{R}^2 \setminus \Omega$.

The other very tricky idea is to use quantitatively that all the open sets of the partition cannot be very close to disks (packing density) (see Blind [**8**]).

The inequality obtained by Bourgain is the following (see (37) in [**11**]) as $k \to +\infty$, is that for any $\delta \in (0, \delta_0)$

$$\frac{\mathfrak{L}_k(\Omega)}{k} \geq (1 + o(1))\lambda(\mathrm{Disk}_1)A(\Omega)^{-1} \times b(\delta) \tag{4.2}$$

where

$$b(\delta) := (1 + 250\delta^{-3})(\frac{\pi}{\sqrt{12}}(1-\delta)^{-2} + 250\delta^{-3})^{-1}\,.$$

and $\delta_0 \in (0,1)$ is computed with the help of the packing condition. This condition reads

$$\frac{\delta_0^3}{250} = (\frac{1-\delta_0}{p})^2 - 1\,,$$

where p is a packing constant determined by Blind [**8**] ($p \sim 0.743$).

But for $\delta > 0$ small enough, we get $b(\delta) > 1$ (as a consequence of $\frac{\pi}{\sqrt{12}} < 1$), hence Bourgain has improved what was obtained via Faber-Krahn (see (3.9)).

As also observed by Steinerberger, one gets

$$\frac{\lambda(\mathrm{Hexa}_1)}{\lambda(\mathrm{Disk}_1)} \geq \sup_{\delta \in (0,\delta_0)} b(\delta) > 1\,,$$

which gives a limit for any improvement of the estimate.

In any case, we have

$$\liminf_{k \to +\infty} \frac{\mathfrak{L}_k(\Omega)}{k} \geq \lambda(\mathrm{Disk}_1)A(\Omega)^{-1} \times \sup_{\delta \in (0,\delta_0)} b(\delta)\,. \tag{4.3}$$

4.3. The uncertainty principle by S. Steinerberger. To explain this principle, we associate with a partition $\mathcal{D} = (\Omega_i)$ of Ω

$$D(\Omega_i) = 1 - \frac{\min_j A(\Omega_j)}{A(\Omega_i)}\,.$$

We also need to define for an open set D with finite area, the Fraenkel asymmetry of D:

$$\mathcal{A}(D) = \inf_B \frac{A(D \triangle B)}{A(D)}\,,$$

where the infimum is over the balls of same area and where

$$D \triangle B = (D \setminus B) \cup (B \setminus D)\,.$$

Steinerberger's uncertainty principle reads:

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THEOREM 4.2.
There exists a universal constant $c > 0$, and a $k_0(\Omega)$ such that for each k-partition of Ω: $\mathcal{D} = (\Omega_i)_{i=1,\dots,k}$, with $k \geq k_0(\Omega)$,

$$\sum_i (D(\Omega_i) + \mathcal{A}(\Omega_i)) \frac{A(\Omega_i)}{A(\Omega)} \geq c\,. \tag{4.4}$$

4.4. Application to equipartitions of energy λ. Let us show how we recover a lower bound for $\liminf_{k\to+\infty} (\mathfrak{L}_k(\Omega)/k)$ improving (3.9) asymptotically. We consider a k-equipartition of energy λ. We recall from [**3**] that an equipartition is a strong partition for which the ground state energy in each open set D_i is the same. In particular, nodal partitions and minimal partitions for $\mathfrak{L}_k$ are typical examples of equipartitions. If we assume that $k \geq k_0(\Omega)$, the uncertainty principle says that its is enough to consider two cases.

We first assume that

$$\sum_i D(\Omega_i) \frac{A(\Omega_i)}{A(\Omega)} \geq \frac{c}{2}\,.$$

We can rewrite this inequality in the form:

$$k \inf_j A(\Omega_j) \leq (1 - \frac{c}{2}) A(\Omega)\,.$$

After implementation of Faber-Krahn, we obtain

$$\frac{k}{\lambda} \lambda(Disk_1) \leq (1 - \frac{c}{2}) A(\Omega)\,. \tag{4.5}$$

We now assume that

$$\sum_i \mathcal{A}(\Omega_i) \frac{A(\Omega_i)}{A(\Omega)} \geq \frac{c}{2}\,.$$

This assumption implies, using that $\mathcal{A}(\Omega_i) \leq 2$,

$$A\left(\cup_{\{\mathcal{A}(\Omega_i) \geq \frac{c}{6}\}} \Omega_i\right) \geq \frac{c}{6} A(\Omega)\,. \tag{4.6}$$

The role of $\mathcal{A}$ can be understood from the following inequality due to Brasco, De Philippis, and Velichkov [**13**]:
There exists $C > 0$ such that, for any open set ω with finite area,

$$A(\omega)\lambda(\omega) - \lambda(Disk_1) \geq C \mathcal{A}(\omega)^2 \lambda(Disk_1)\,. \tag{4.7}$$

If we apply this inequality with $\omega = \Omega_i$, it reads

$$A(\Omega_i)\lambda - \lambda(Disk_1) \geq C \mathcal{A}(\Omega_i)^2 \lambda(Disk_1)\,.$$

Hence we get for any i such that $\mathcal{A}(\Omega_i) \geq \frac{c}{6}$, the inequality

$$\lambda(Disk_1)(1 + \frac{Cc^2}{36}) \leq A(\Omega_i)\lambda\,, \tag{4.8}$$

which is an improvement of Faber-Krahn for these Ω_i's.

Summing over i and using (4.6) leads to

$$\frac{k}{\lambda} \lambda(Disk_1) \leq (1 + \frac{Cc^2}{36})^{-1} A(\Omega) \left(1 + (1 - \frac{c}{6}) \frac{Cc^2}{36}\right)\,,$$

and finally to

$$\frac{k}{\lambda} \lambda(Disk_1) \leq \left(1 - \frac{Cc^3}{216 + 6Cc^2}\right) A(\Omega)\,. \tag{4.9}$$

Putting (4.5) and (4.8) together, we obtain that for $k \geq k_0(\Omega)$ (as assumed from the beginning) the k-partition satisfies

$$\frac{k}{\lambda}\lambda(Disk_1) \leq \max\left((1-\frac{c}{2}),(1-\frac{Cc^3}{216+6Cc^2})\right) A(\Omega)\,. \tag{4.10}$$

If we apply this to minimal partitions ($\lambda = \mathfrak{L}_k(\Omega)$), this reads

$$\lambda(Disk_1) \leq \max\left((1-\frac{c}{2}),(1-\frac{Cc^3}{216+6Cc^2})\right) A(\Omega) \liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}\,. \tag{4.11}$$

Hence S. Steinerberger recovers Bourgain's improvement (4.3) with a not explicit constant[2].

REMARK 4.3. *Steinerberger obtains also a similar lower bound to* (4.11) *for* $\liminf_{k\to+\infty} \frac{\mathfrak{L}_{k,1}(\Omega)}{k}$ *using a convexity argument.*

5. Considerations around rectangles

The detailed analysis of the spectrum of the Dirichlet Laplacian in a rectangle is basic in Pleijel's paper [**25**]. As mentioned in [**17**], other results have been previously obtained in the PHD of A. Stern [**30**], defended in 1924. Other aspects relative to spectral minimal partitions appear in [**23**]. Take $\mathcal{R}(a,b) = (0,a\pi)\times(0,b\pi)$. The eigenvalues are given by

$$\hat{\lambda}_{m,n} = (\frac{m^2}{a^2}+\frac{n^2}{b^2})\,,$$

with a corresponding basis of eigenfunctions given by

$$\phi_{m,n}(x,y) = \sin\frac{mx}{a}\,\sin\frac{ny}{b}\,.$$

If it is easy to determine the Courant sharp cases when b^2/a^2 is irrational (see for example [**23**]). The rational case is more difficult. Pleijel claims in [**25**] that in the case of the square it is Courant sharp if and only if $k = 1, 2, 4$. The exclusion of $k = 5, 7, 9$ is however not justified (the author refers indeed to Courant-Hilbert [**17**] where only pictures are presented, actually taken from the old book (1891) by Pockels [**26**]). This can actually be controlled by an explicit computation of the nodal sets of each combination ($\theta \in [0,\pi)$):

$$\Phi_{m,n,\theta} := \cos\theta\phi_{m,n} + \sin\theta\phi_{n,m}$$

for $(m,n) = (1,3)\,,\ (1,4)\,,$ and $(2,3)$.

In this context the following guess could be natural:
Suppose that $\hat{\lambda}_{m,n}$ *has multiplicity* $\mathfrak{m}(m,n)$. *Let* $\mu_{\max}(u)$ *be the maximum of the number of nodal domains of the eigenfunctions in the eigenspace associated with* $\hat{\lambda}_{m,n}$.

$$\mu_{\max} = \sup_j (m_j n_j)\,,$$

where the sup is computed over the pairs (m_j, n_j) *such that*

$$\hat{\lambda}_{m_j,n_j} = \hat{\lambda}_{m,n}\,.$$

The problem is not easy because one has to consider, in the case of degenerate eigenvalues, linear combinations of the canonical eigenfunctions associated with

[2] At least C in (4.7) is not explicit.

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the $\hat{\lambda}_{m,n}$. Actually, as stated above, the guess is wrong. As observed by Pleijel [**25**], the eigenfunction $\Phi_{1,3,\frac{3\pi}{4}}$ corresponding to the fifth eigenvalue has four nodal domains delimited by the two diagonals, and $\mu_{max} = 3$. More generally one can consider $u_k := \Phi_{1,3,\frac{3\pi}{4}}(2^k x, 2^k y)$ to get an eigenfunction associated with the eigenvalue $\lambda_{n(k)} = \hat{\lambda}_{2^k,3\cdot 2^k} = 10 \cdot 4^k$ with 4^{k+1} nodal domains. The corresponding quotient $\frac{\mu(u_k)}{n(k)}$ is asymptotic to $\frac{8}{5\pi}$. This does not contradict the Polterovich conjecture. Note also that for each number K, there is an eigenfunction u with $\mu(u) \geq K$. Finally let us mention that counterexamples to a similar guess in the Neumann case can be found in [**26**].

Pleijel's constant.
We consider for each Ω and each orthonormal basis $\mathcal{B}_\Omega := (u_n)$ of the Dirichlet Laplacian:

$$Pl(\Omega, \mathcal{B}_\Omega) = \limsup_{n\to+\infty} \frac{\mu_n^{\Omega,\mathcal{B}}}{n}\,, \tag{5.1}$$

where $\mu_n^{\Omega,\mathcal{B}}$ denotes the number of nodal domains of u_n.

The reference to $\mathcal{B}$ is only needed in the case when the Laplacian has a infinite sequence of multiple eigenvalues. We then define:

$$Pl(\Omega) = \sup_{\mathcal{B}_\Omega} Pl(\Omega, \mathcal{B}_\Omega)\,. \tag{5.2}$$

Now the question arises how and whether $Pl(\Omega)$ depends on Ω. Note that $Pl(\Omega) = Pl(T\Omega)$ where T denotes scaling or rotation, reflection, translation.

It is not even clear that $\mu_n^{\Omega,\mathcal{B}}$ tends for every Ω to infinity, see [**24**]. The Pleijel constant could be defined as

$$Pl = \sup_{\Omega} Pl(\Omega)\,, \tag{5.3}$$

and it is not at all clear that a maximizing pair $(\Omega, \mathcal{B}_\Omega)$ exists. (The square or more generally rectangles might be good candidates as mentioned above.) It would be interesting to find those domains, for which it is possible to calculate $Pl(\Omega)$.

We finally recall (cf [**9**] and [**27**]) that

PROPOSITION 5.1. *Let us assume that b^2/a^2 is irrational.*

$$Pl(\mathcal{R}(a,b)) = \frac{2}{\pi}\,. \tag{5.4}$$

Proof
It suffices to consider $\mathcal{R}(\pi, b\pi)$ for irrational b^2. Since b^2 is irrational the eigenvalues are simple and

$$\mu(\phi_{m,n}) = mn\,. \tag{5.5}$$

Weyl asymptotics tells us that with $\lambda = \hat{\lambda}_{m,n}$:

$$k(m,n) := \#\{(\tilde{m},\tilde{n}) : \hat{\lambda}_{\tilde{m},\tilde{n}}(b) < \lambda\} = \frac{b\pi}{4}(m^2 + n^2/b^2) + o(\lambda)\,. \tag{5.6}$$

We have

$$\lambda_{k(m,n)+1} = \hat{\lambda}_{m,n}\,.$$

We observe that $\mu(\phi_{n,m})/\hat{k}(n,m)$ is asymptotically given by

$$P(m,n;b) := \frac{4mn}{\pi(m^2b + n^2/b)} \leq \frac{2}{\pi}\,. \tag{5.7}$$

Next we take a sequence (m_k, n_k) such that $b = \lim_{k\to\infty} \frac{n_k}{m_k}$ with $m_k \to +\infty$. We observe that

$$\lim_{k\to+\infty} P(m_k, n_k, b) = \frac{2}{\pi}\,. \tag{5.8}$$

This proves the proposition using the sequence of eigenfunctions ϕ_{m_k,n_k}.

REMARK 5.2. *We have consequently*

$$Pl \geq \frac{2}{\pi}\,, \tag{5.9}$$

the conjecture being that one actually has the equality.

The case when $b^2/a^2 \in \mathbb{Q}$ depends on the discussion at the beginning of the section. We only know that

$$Pl(R(a,b)) \geq \frac{2}{\pi}\,, \tag{5.10}$$

6. Looking for a class $\mathcal{O}^{\#}$.

We now start the discussion on tentative choices of the classes $\mathcal{O}_k^{\sharp}$ (see Definition 3.3).

6.1. Bipartite partitions. If we think that only nodal partitions are involved in Pleijel's theorem, it could be natural to consider as class $\mathcal{O}_k^{\sharp}$ the class $\mathcal{O}_k^{bp}$ of the bipartite strong regular connected k-partitions $\mathcal{D} = (D_1, \cdots, D_k)$. Note that there is some arbitrariness in the definition but "strong" is necessary to define a bipartite partition.

DEFINITION 6.1.

$$\mathfrak{L}_k^{bp}(\Omega) := \inf_{\mathcal{D}\in\mathcal{O}_k^{bp,str}} \max \lambda(D_i)\,. \tag{6.1}$$

Although this definition is natural, all what has been established relatively to $\mathfrak{L}_k(\Omega)$ is unclear or at least unproved in the case of this $\mathfrak{L}_k^{bp}(\Omega)$.

By definition, we know that $\mathfrak{L}_k^{bp}(\Omega) \leq L_k(\Omega)$. If the inequality is strict the infimum cannot by definition correspond to a nodal partition. If we want this notion to be helpful for improving Pleijel's constant, it is natural to first ask if $\mathfrak{L}_k^{bp}(\Omega) > \mathfrak{L}_k(\Omega)$, at least for k large. However we will show

PROPOSITION 6.2. *Suppose that Ω is simply connected. Then*

$$\mathfrak{L}_k^{bp}(\Omega) = \mathfrak{L}_k(\Omega)\,. \tag{6.2}$$

Hence this class which could a priori appear to be a natural candidate for $\mathcal{O}^{\sharp}$ does not lead to any improvement of the hexagonal conjecture for Pleijel's theorem.

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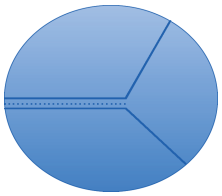

FIGURE 2. Scheme of the construction for the Mercedes Star

6.2. Proof of Proposition 6.2. Particular case.
Suppose that $\Omega \subset \mathbb{R}^2$, $k \geq 2$ and consider a minimal k-partition $\mathcal{D} = \{D_i, \dots, D_k\}$ which is not bipartite. We first prove the proposition in a particular case.

LEMMA 6.3. *We assume that Ω is simply connected and that*

$$\#\{\cup \partial D_i\} = 1\,. \tag{6.3}$$

Then there is a sequence of bipartite k-partitions $\widehat{\mathcal{D}}_k(\epsilon) = \{\widehat{D}_1(\epsilon), \dots, \widehat{D}_k(\epsilon)\}$ of Ω with the property that

$$\Lambda(\widehat{\mathcal{D}}_k(\epsilon)) \to \mathfrak{L}_k(\Omega),\ j = 1, \dots, k. \tag{6.4}$$

For $\epsilon > 0$, we define for any element of the partition

$$D_i(\epsilon) = \{x \in D_i \mid \mathrm{dist}(x, \partial D_i) > \epsilon\}. \tag{6.5}$$

For $\epsilon > 0$ small enough all the $D_i(\epsilon)$ are non empty and connected.

We also define a tubular ϵ-neighborhood of $\partial\Omega \cup N(\mathcal{D}))$ in Ω :

$$\mathcal{S}^\epsilon = \{x \in \Omega, d(x, \partial\Omega \cup N(\mathcal{D})) < \epsilon\}$$

$\mathcal{S}^\epsilon$ is connected due to Assumption (6.3).

Now as ϵ tends to zero, $A(\mathcal{S}^\epsilon) \to 0$. We consider the k-partition $\widehat{\mathcal{D}}(\epsilon)$ defined by

$$\widehat{D}_1(\epsilon) = D_1 \cup \mathcal{S}^\epsilon\,,\ \widehat{D}_i(\epsilon) = D_i(\epsilon)\,,\ \forall i > 1\,.$$

This gives a connected open k-partition of Ω with the following property:

$$\lambda(\widehat{D}_1(\epsilon)) < \lambda(D_1)\,,\ \lim_{\epsilon \to 0} \lambda(\widehat{D}_i(\epsilon)) = \lambda(D_i)\,,\ \forall i > 1\,.$$

□

Figure 2 describes the construction in the case of the disk, assuming (see [**23**], [**20**]) that the minimal 3-partition is the Mercedes-star.

General case.
We now give the proof in the general case. Considering the previous discussion, we can distinguish two cases for our minimal k-partition $\mathcal{D}$.

(i) $N(\mathcal{D})$ does not meet $\partial\Omega$
(ii) $N(\mathcal{D}) \cap \partial\Omega \neq \emptyset$.

In the first case, after relabeling we can call D_1 the unique element of the partition whose boundary touches $\partial\Omega$. We follow the previous discussion and define $S^{(1)}(\epsilon)$ the connected component of the set S^ϵ containing $\partial D_1 \cap \Omega$. The first element of the approximating k-partition is then

$$\widehat{D}_1(\epsilon) := D_1 \cup S^{(1)}(\epsilon)\,.$$

In the second case, after relabeling, we can take as D_1 one element of the partition such that $\partial D_1 \cap \partial\Omega \neq \emptyset$ and as before introduce $\widehat{D}_1(\epsilon)$ as before but with $S^{(1)}(\epsilon)$ the connected component of the set S^ϵ containing $\partial\Omega$.

We now consider the connected components $\Omega \backslash \overline{\widehat{D}_1(\epsilon)}$. Many of them are simply $D_j(\epsilon)$ for $j > 1$. We keep these open sets as elements of our new partition. Other components contain more than one D_ℓ. If we denote by $\Omega^{(\ell)}(\epsilon)$ such a component, we observe that we are necessarily in case (i) of the previous discussion with $\Omega^{(\ell)}(\epsilon)$ replacing Ω. Only one $D_k(\epsilon)$ inside $\Omega^{(\ell)}$ can have its boundary touching $\overline{\widehat{D}_1(\epsilon)}$. We can iterate inside $\Omega^{(\ell)}(\epsilon)$ what we have done in Ω and the procedure will stop after a finite number of iterations.

REMARK 6.4. *The case when Ω is not simply connected can be handled similarly.*

6.3. Almost nodal partitions. Here is a new try for a definition of $\mathcal{O}^\sharp$ in order to have a flexible notion of partitions which are close with nodal partitions. We assume that Ω is regular and simply connected.

We will say that a k-partition $\mathcal{D}$ of Ω of energy $\Lambda(\mathcal{D})$ is almost nodal, if there is a connected open set $\Omega' \subset \Omega$ and a $(k-1)$-subpartition $\mathcal{D}'$ of $\mathcal{D}$ such that $\mathcal{D}'$ is a nodal partition of Ω' of energy $\Lambda(\mathcal{D})$. Of course a nodal partition is almost nodal. The first useful observation is that for any k there exists always an almost nodal k-partition. The proof is obtained using a sufficiently thin "square" $(k-1)$-partition in Ω and completing by the complement in Ω of the closure of the union of the preceding squares. See the right subfigure of Figure 1. Denoting by $\mathcal{O}_k^{a.n}$ the set of the almost nodal partitions, we introduce

$$\mathfrak{L}_k^{a.n}(\Omega) = \inf_{\mathcal{D}\in\mathcal{O}_k^{a.n,j}} \Lambda(\mathcal{D})\,. \tag{6.6}$$

Of course, we have

$$\mathfrak{L}_k(\Omega) \leq \mathfrak{L}_k^{a.n}(\Omega) \leq L_k(\Omega)\,. \tag{6.7}$$

The next point is to observe, by the same proof giving (3.13) but playing with the square tiling (see Figure 1), that

$$A(\Omega)\limsup_{k\to+\infty} \frac{\mathfrak{L}_k^{a.n}(\Omega)}{k} \leq \lambda(Sq_1)\,. \tag{6.8}$$

Again the question arises about the asymptotic behavior of $\liminf_{k\to+\infty} \frac{\mathfrak{L}_k^{a.n}(\Omega)}{k}$. Unfortunately there are good reasons to think that we can improve (6.8) by proving

$$A(\Omega)\limsup_{k\to+\infty} \frac{\mathfrak{L}_k^{a.n}(\Omega)}{k} \leq \lambda(Hexa_1)\,. \tag{6.9}$$

We just give an heuristical hint. For k large, we try to "almost" fill Ω with a maximal number of $(k-1)$ adjacent isometric regular hexagons D_i $(i = 1,\dots,k-1)$. For k large, they should have an area of order $A(\Omega)/k$ and an energy of order $k\lambda(Hexa_1)/A(\Omega)$. and we complete the partition by taking as D_k the complement in Ω of $\overline{\cup_{i=1}^{k-1} D_i}$. We can in addition have the property that $\lambda(D_k) \leq \lambda(D_1)$ (one way is to start with k adjacent regular hexagons and to delete one). Then we construct our set Ω'_{k-1} by subtracting cracks (edges of some of the hexagons) from $\mathrm{Int}\,(\overline{\cup_{i=1}^{k-1} D_i})$ in such a way that $(D_1,\dots,D_{k-1})$ becomes a nodal $(k-1)$-partition

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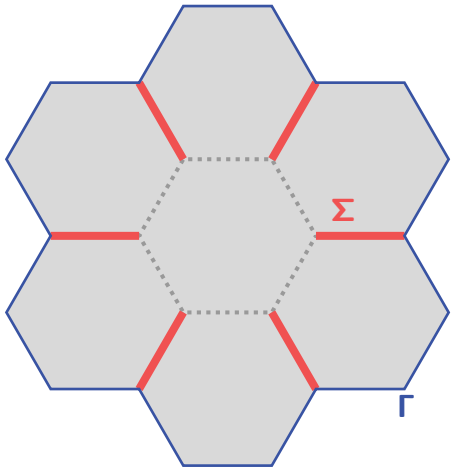

FIGURE 3. Scheme of the construction of the cracks for $(k-1)=7$.

of Ω'_{k-1} (see Figure 3). Such a construction is detailed in [**12**], when exploring the consequences of the hexagonal conjecture. This conjecture would actually impose that this is the nodal partition of a Courant sharp eigenfunction but we do not need it at this stage. Then the partition is almost nodal and asymptotically of energy $k\lambda(Hexa_1)/A(\Omega)$.

Actually, starting directly from a minimal k-partition $\mathcal{D}=(D_1,\dots,D_k)$ and proceeding as before with the $(k-1)$ first elements, one can add curved segments belonging to the boundary of the partition such that we get a nodal partition. Here we use a property observed in [**23**] (Proof of Proposition 8.3) (see also Corollary 2.11 in [**12**]). This will directly lead to the stronger equality $\mathfrak{L}_k^{a.n}(\Omega)=\mathfrak{L}_k(\Omega)$.

Of course, one could think that by imposing more regularity on the partition and on Ω', one can eliminate this kind of examples. But as in the previous subsection, an approximation of the cracks by fine tubes could probably be used for getting the same inequality. This we have not checked and will be much more technical than for the proof of Proposition 6.2.

Hence the class of almost nodal partitions is probably too large for getting a higher infimum.

6.4. Conclusion. In conclusion, we were looking for smaller classes of partitions containing nodal partitions with the hope to give some justification for the Polterovich conjecture. We have shown that two natural choices do not give a confirmation of this conjecture as initially expected.

7. Pleijel's Theorem for Aharonov-Bohm operators and application to minimal partitions

7.1. The Aharonov-Bohm approach. Let us recall some definitions and results about the Aharonov-Bohm Hamiltonian in an open set Ω (for short $\mathbf{AB}X$-Hamiltonian) with a singularity at $X\in\Omega$ as introduced in [**22**]. We denote by $X=(x_0,y_0)$ the coordinates of the pole and consider the magnetic potential with

flux at X: $\Phi = \pi$, defined in $\dot{\Omega_X} = \Omega \setminus \{X\}$:

$$\mathbf{A}^X(x,y) = (A_1^X(x,y), A_2^X(x,y)) = \frac{1}{2}\left(-\frac{y-y_0}{r^2}, \frac{x-x_0}{r^2}\right). \tag{7.1}$$

The $\mathbf{AB}X$-Hamiltonian is defined by considering the Friedrichs extension starting from $C_0^\infty(\dot{\Omega}_X)$ and the associated differential operator is

$$-\Delta_{\mathbf{A}^X} := (D_x - A_1^X)^2 + (D_y - A_2^X)^2 \text{ with } D_x = -i\partial_x \text{ and } D_y = -i\partial_y. \tag{7.2}$$

Let K_X be the antilinear operator $K_X = e^{i\theta_X}\ \Gamma$, with $(x-x_0) + i(y-y_0) = \sqrt{|x-x_0|^2 + |y-y_0|^2}\, e^{i\theta_X}$, θ_X such that $d\theta_X = 2\mathbf{A}^X$, and where Γ is the complex conjugation operator $\Gamma u = \bar{u}$. A function u is called K_X-real, if $K_X u = u$. The operator $-\Delta_{\mathbf{A}^X}$ is preserving the K_X-real functions and we can consider a basis of K_X-real eigenfunctions. Hence we only analyze the restriction of the $\mathbf{AB}X$-Hamiltonian to the K_X-real space $L^2_{K_X}$ where

$$L^2_{K_X}(\dot{\Omega}_X) = \{u \in L^2(\dot{\Omega}_X)\ ,\ K_X\, u = u\}.$$

It was shown in [**22**] and [**1**] that the nodal set of such a K_X real eigenfunction has the same structure as the nodal set of an eigenfunction of the Laplacian except that an odd number of half-lines meet at X. In particular, for a K_X-real groundstate (one pole), one can prove [**22**] that the nodal set consists of one line joining the pole and the boundary.

Extension to many poles

We can extend this construction in the case of a configuration with ℓ distinct points $X_1, \ldots, X_\ell$ (putting a flux π at each of these points). We just take as magnetic potential

$$\mathbf{A}^{\mathbf{X}} = \sum_{j=1}^{\ell} \mathbf{A}^{X_j}\ ,\ \text{where } \mathbf{X} = (X_1, \ldots, X_\ell).$$

We can also construct the antilinear operator $K_{\mathbf{X}}$, where θ_X is replaced by a multivalued-function $\phi_{\mathbf{X}}$ such that $d\phi_X = 2\mathbf{A}^{\mathbf{X}}$. We can then consider the real subspace of the $K_{\mathbf{X}}$-real functions in $L^2_{K_{\mathbf{X}}}(\dot{\Omega}_{\mathbf{X}})$. It has been shown that the $K_{\mathbf{X}}$-real eigenfunctions have a regular nodal set (like the eigenfunctions of the Dirichlet Laplacian) with the exception that at each singular point X_j $(j = 1, \ldots, \ell)$ an odd number of half-lines meet. We recall the following theorem which is the most interesting part of the magnetic characterization of the minimal partitions given in [**21**]:

THEOREM 7.1.
Let Ω be simply connected. If $\mathcal{D}$ is a k-minimal partition of Ω, then, by choosing[3] *$(X_1, \ldots, X_\ell) = X^{odd}(N(\mathcal{D}))$, $\mathcal{D}$ is the nodal partition of some k-th $K_{\mathbf{X}}$-real eigenfunction of the Aharonov-Bohm Laplacian associated with $\dot{\Omega}_{\mathbf{X}}$.*

7.2. Analysis of the critical sets in the large limit case. We first consider the case of one pole X. We look at a sequence of K_X-real eigenfunctions and follow the proof of Pleijel on the number of nodal domains. We observe that the part devoted to the lower bound works along the same lines and the way we shall meet $\mathfrak{L}_k(\Omega)$ is unchanged. When using the Weyl formula, we observe that only a lower bound of the counting function is used (see around (3.4)). If the distance of X to the boundary is larger than ϵ, we introduce a disk $D(X,\epsilon)$ of radius ϵ around

[3] We recall that $X(N)$ is defined after Definition 2.2.

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X ($\epsilon > 0$) and consider the Dirichlet magnetic Laplacian in $\Omega \setminus \bar{D}(X, \epsilon)$. For the X at the distance less than ϵ of the boundary, we look at the magnetic Laplacian on Ω minus a (2ϵ)-tubular neighborhood of the boundary. In the two cases, we get an elliptic operator where the main term is the Laplacian $-\Delta$. Hence we can combine the monotonicity of the Dirichlet problem with respect to the variation of the domain to the use of the standard Weyl formula (see (3.4)) to get (uniformly for X in Ω), an estimate for the counting function $N_X(\lambda)$ of $-\Delta_{\mathbf{A}^{\mathbf{X}}}$ in the following way:
There exists a constant $C > 0$ such that, for any $\epsilon > 0$, as $\lambda \to +\infty$,

$$N_X(\lambda) \geq \frac{1}{4\pi}(1 - C\epsilon)A(\Omega)\,\lambda + o(\lambda)\,.$$

Hence, for any $\epsilon > 0$, any $X \in \Omega$,

$$\limsup_{n\to+\infty} \mu(\phi_n^X)/n \leq (1 + C\epsilon)\frac{4\pi}{A(\Omega)\liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}}\,.$$

Taking the limit $\epsilon \to 0$, we get:

$$\limsup_{n\to+\infty} \mu(\phi_n^X)/n \leq \frac{4\pi}{A(\Omega)\liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}}\,. \tag{7.3}$$

Till now X was fixed. But everything being uniform with respect to X, we can also consider a sequence $\phi_n^{X_n}$ corresponding to the n-th eigenvalue of $-\Delta_{\mathbf{A}_{X_n}}$.

Suppose that for a subsequence k_j, we have a k_j-minimal partition with only one pole X_j in Ω. Let $\phi_{k_j}^{X_j}$ the corresponding eigenfunction. Hence, we are in a Courant sharp situation. The inequality above leads this time (possibly after extraction of a subsequence) to

$$1 \leq \frac{4\pi}{A(\Omega)\liminf_{k\to+\infty} \frac{\mathfrak{L}_k(\Omega)}{k}} \leq \nu_{Pl} \sim 0.691\,.$$

Hence a contradiction.

We can play the same game with more than one pole and get as consequence:

PROPOSITION 7.2. *If for $k \in \mathbb{N}$, $\mathcal{D}_k$ denotes a minimal k-partition, then*

$$\lim_{k\to+\infty} \#X^{odd}(N(\mathcal{D}_k)) = +\infty\,. \tag{7.4}$$

Proof.
Suppose indeed that this cardinality does not tend to $+\infty$. We can then extract a subsequence such that this cardinality is finite. After new extractions of a subsequence, we can assume that this cardinality is fixed and that each critical point tends to a limiting point, which could be either at the boundary $\partial\Omega$ or in Ω. We apply Theorem 7.1 and consider the associated Aharonov-Bohm hamiltonians, whose poles are these odd critical points. We can then find a finite number of disks of radius ϵ centered at these limiting poles such that all the poles are contained in these balls for k large enough. Then outside of these balls the potential A^X and the derivatives are bounded by a uniform bound (depending on ϵ) and the same construction works and leads to a contradiction.

REMARK 7.3. *We recall that an upper bound for* $\#X(N(\mathcal{D}_k))$ *is given in* [**19**] *(case with no holes) by using Euler's formula:*

$$\#X^{odd}(N(\mathcal{D}_k)) \leq 2k-4\,. \tag{7.5}$$

On the other hand, the hexagonal conjecture for the asymptotic number of odd critical points of a k-minimal partition reads as follows:

$$\lim_{k\to+\infty} \frac{\#X^{odd}(N(\mathcal{D}_k))}{k} = 2\,. \tag{7.6}$$

Hence there are good reasons to believe that the upper bound (7.5) *is asymptotically optimal.*

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Increasing stability for near field from the scattering amplitude

Victor Isakov

Abstract. We obtain stability estimates for the near field of a radiating solution of the Helmholtz equation from the far field (scattering amplitude). This estimates contain the best possible Lipschitz term, a Hölder term, and terms which decay as powers of the frequency k for large k under some a priori bounds. These estimates contain only explicit constants and show increasing stability of recovery of the near field from scattering amplitude with growing k. Proofs are elementary and are based on new explicit bounds for Hankel functions. We give first applications to increasing stability in (linearized) inverse scattering by obstacles.

1. Introduction

Many inverse problems are known to be severely ill-posed. This makes it extremely difficult to design reliable reconstruction algorithms and dramatically restricts their resolution in practice. However, in some cases, it has been observed numerically that the stability increases with respect to some parameter such as the wave number (or energy). Ill-posedness occurs at the stage of the continuation of solutions of partial differential equations from observation set toward an obstacle. Several rigorous justifications of the increasing stability phenomena in the Cauchy (or continuation) problem in different settings were obtained by Isakov *et al* [**HI**, **I2**, **IK**, **AI**]. These justifications are in form of conditional stability estimates which are getting nearly Lipschitz when the wave number k is getting large.

For increasing stability for the Schrödinger potential from the Dirichlet-to-Neumann map we refer to [**I3**], [**IN**], [**INUW**], and [**IW**]. As a an important example of (at least generically and locally) well-posed inverse scattering problem we mention the inverse backscattering problem [**ER**].

We consider a solution u to the Helmholtz equation

$$(\Delta + k^2)u = 0 \text{ in } \mathbb{R}^3 \setminus \bar{D}, \tag{1.1}$$

satisfying the Sommerfeld radiation condition

$$lim\ r(\partial_r u - iku)(x) = 0 \text{ as } r \to \infty. \tag{1.2}$$

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Here $r = |x|$. As well known [**CK**], [**LP**], [**T**] the relations (1.1), (1.2) imply that

$$u(x) = \frac{e^{ikr}}{r} A(\sigma) + O(r^{-2}),$$

where $\sigma = r^{-1}x$ and $A(\sigma)$ is the so called scattering amplitude (or pattern). We are interested in recovery of u from A. It is known that A is a (real) analytic function on the unit sphere. Uniqueness of u follows from well know Rellich Theorem. Our main goal is to study stability of this recovery.

In this paper we will denote by B_R the ball $\{x : |x| < R\}$ in $\mathbb{R}^3$.

To state our results we use the complete orthonormal base in $L^2(B_1)$ formed of spherical harmonics $Y_n^m(\sigma), n = 0, 1, 2, \dots, m = -n, \dots, 0, \dots, n$. Let $A \in L^2(B_R)$ and $a_{m,n}$ be the coefficients of the expansion of A with respect to Y_n^m, i.e., $A = \sum_{n,m} a_{m,n} Y_n^m$. For brevity, we introduce

$$Y_n(\cdot; A) = a_n^{-1} \sum_{m=-n,\dots,n} a_{m,n} Y_n^m, a_n = (\sum_{m=-n,\dots,n} |a_{m,n}|^2)^{\frac{1}{2}}$$

and $Y_n(\cdot; A) = 0$ when $a_n = 0$, then

$$A(\sigma) = \sum_{n=0}^{\infty} a_n Y_n(\sigma; A). \tag{1.3}$$

Observe that $\|A\|^2_{(0)} = \sum_{n=0}^{\infty} |a_n|^2$. As known [**CK**], [**T**],

$$u(x) = \sum_{n=0}^{\infty} u_n(r) Y_n(\sigma; A), \text{ where } u_n(r) = kia_n h_n^{(1)}(kr), \tag{1.4}$$

where $h_n^{(1)}$ is the (spherical) Hankel function.

For a function u with the expansion (1.4) we will use the following (natural) Sobolev norm

$$\|u\|^2_{(l)}(\partial B_R) = R^2 \sum_{m=0}^{l} \sum_{n=0}^{\infty} (\frac{n}{R})^{2m} |u_n(R)|^2. \tag{1.5}$$

We let $\varepsilon_1^2 = \sum_{n=0}^{N} |a_n|^2, \varepsilon_2^2 = \sum_{n=N+1}^{\infty} |a_n|^2$.

Now we state our main results where we chosen $N = [\sqrt{kR}]$ and $E = -log\varepsilon_2$. Here $[a]$ is the entire part of a. We consider $u \in H^2(B_\rho \setminus \bar{B}_R)$ for any $\rho > R$.

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THEOREM 1.1. *Assume that* $2 \leq kR$.
Then we have the following stability estimates

$$\|u\|^2_{(0)}(\partial B_R) \leq \frac{2e^2}{\pi}\varepsilon_1^2 + \frac{2}{\pi}e^{\frac{2}{R}}\varepsilon_2 + R^2\frac{M_1^2}{E+k}, \tag{1.6}$$

and

$$\|u\|^2_{(0)}(\partial B_R) \leq \frac{2e^2}{\pi}\varepsilon_1^2 + \sqrt{\frac{2R}{\pi k}}e^{\frac{1}{R}}M_1\varepsilon_2^{\frac{1}{2}} + R^2\frac{M_1^2}{E+k}, \tag{1.7}$$

where $M_1 = \|u\|_{(1)}(\partial B_R)$.

THEOREM 1.2. *Assume that* $2 \leq kR$.
Then we have the following stability estimate:

$$\|\partial_r u\|^2_{(0)}(\partial B_R) \leq$$

$$\frac{e^2}{\pi}(3+\sqrt{5})k^2\varepsilon_1^2 + k^2e^{\frac{2}{R}}\varepsilon_2 + R^2\frac{M_2^2}{E+k-2\sqrt{E+k}+1}, \tag{1.8}$$

where $M_2 = \|\partial_r u\|_{(1)}(\partial B_R)$.

From estimates (1.6), (1.7) it is obvious that the stability behaves more like Lipschitz type when k is large. Indeed, the second and third terms on the right side (1.7) go to zero as powers of k, which quantifies the increasing stability. We observe that the bounds (1.6), (1.7), (1.8) are so called conditional stability estimates: they guarantee stability under a priori constrains of higher norms of solutions. Due to ill-posedness of recovery of u from A ([**B**], [**CK**],[**I**], [**T**]) stability estimates are impossible without such constraints.

Known stability estimates for u from its scattering amplitude [**B**], [**I**], [**T**] are of logarithmic type, contain unknown constants, and do not indicate increasing stability for larger k.

Our proofs are using well known expression (1.4) of u via the expansion (1.3) of the scattering amplitude as the series in spherical harmonics. The crucial step is explicit upper bounds for the Hankel functions $h_n^{(1)}(t)$ given by Lemmas 2.1, 2.3 with surprisingly short and elementary proofs. Theory of Bessel and Hankel functions abounds with basic, but hard open questions (about sharp maxima, zeros etc) [**W**]. While some bounds (similar to Lemma 2.2) and asymptotic behaviour of these functions are well known, explicit bounds when $0 < t < n$ are only partially available and constants in these bounds are not explicit [**BRV**], Lemma 1, p. 364. Some refined properties of Bessel functions were used by F. John [**J**] to find a crucial example showing growing instability for the continuation of solution to the Helmholtz equation from the unit disk onto its complement in the plane. In [**IK**] by using energy integrals for the Bessel's equation we demonstrated increasing stability of the continuation for the John's example in low frequency zone (which grows with k).

The paper is organized as follows. In Section 2 we will obtain some explicit bounds on Hankel functions $h_n^{(1)}$. In Section 3 we present proofs of Theorem 1.1 and of Theorem 1.2. In Section 4 we give applications to the increasing stability of inverse obstacle scattering problem linearized around a sphere. Finally we discuss challenging open problems and possible further developments.

2. Some bounds of Hankel functions

We will use that

$$h_n^{(1)}(t) = \sqrt{\frac{2}{\pi}} i^n \frac{e^{it}}{t} \sum_{m=0}^{n} (-1)^n \frac{(n+m)!}{m!(n-m)!} \frac{i^m}{(2t)^m}, \tag{2.1}$$

provided $0 < t$. This is a well-known representation of the Hankel function given for example in [**JEL**], p. 142, [**T**], p. 205, [**W**], p. 53.

To prove main results, we need elementary but crucial lemmas.

LEMMA 2.1. *If $n^2 < t$, then*

$$|h_n^{(1)}(t)| < \frac{\sqrt{2}e}{\sqrt{\pi}t}. \tag{2.2}$$

PROOF. Using (2.1) and the triangle inequality we yield

$$|h_n^{(1)}(t)| \le \frac{\sqrt{2}}{\sqrt{\pi}t} \sum_{m=0}^{n} \frac{(n+m)!}{m!(n-m)!} \frac{1}{(2t)^m} \le$$

$$\frac{\sqrt{2}}{\sqrt{\pi}t}(1 + \sum_{m=1}^{n} \frac{(n-m)!}{(n-m)!} \frac{1}{m!} \frac{(n-m+1)\dots n(n+1)\dots(n+m)}{n^m(2n)^m}),$$

where we used the assumption that $n^2 < t$. Since $m \le n$, we have $(n-m+1)\dots n \le n^m$ and $(n+1)\dots(n+m) \le (2n)^m$, so continuing the bounds of $|h_n^{(1)}|$ we obtain

$$|h_n^{(1)}(t)| \le \frac{\sqrt{2}}{\sqrt{\pi}t} \sum_{m=0}^{n} \frac{1}{m!} < \frac{\sqrt{2}e}{\sqrt{\pi}t}.$$

□

LEMMA 2.2. *If $0 < t$, then*

$$|h_n^{(1)}(t)| < \frac{\sqrt{2}}{\sqrt{\pi}t}(1 + \frac{n}{t})^n. \tag{2.3}$$

PROOF. Again using (2.1) and the triangle inequality we yield

$$|h_n^{(1)}(t)| \le \frac{\sqrt{2}}{\sqrt{\pi}t} \sum_{m=0}^{n} \frac{n!}{m!(n-m)!}(n+1)\dots(n+m)\frac{1}{(2t)^m} \le$$

$$\frac{\sqrt{2}}{\sqrt{\pi}t} \sum_{m=0}^{n} \frac{n!}{m!(n-m)!}(\frac{n}{t})^m \le \frac{\sqrt{2}}{\sqrt{\pi}t}(1 + \frac{n}{t})^n,$$

due to the binomial formula. □

Now we similarly obtain bounds for derivatives of the Hankel functions.

LEMMA 2.3. *If $n^2 < t$, then*

$$|\partial_t h_n^{(1)}(t)| < \frac{\sqrt{2}e}{\sqrt{\pi}} \frac{\sqrt{t^2+1}+1}{t^2}. \tag{2.4}$$

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PROOF. Differentiating (2.1) we yield

$$\partial_t h_n^{(1)}(t) = \frac{\sqrt{2}}{\sqrt{\pi}}\frac{e^{it}}{t}\Big(\frac{it-1}{t}\sum_{m=0}^{n}(-1)^n\frac{(n+m)!}{m!(n-m)!}\frac{i^m}{(2t)^m}-$$

$$\sum_{m=1}^{n}(-1)^n\frac{(n+m)!}{m!(n-m)!}\frac{i^m}{(2t)^m}\frac{m}{t}\Big). \tag{2.5}$$

Since $|it-1| = \sqrt{t^2+1}$ as in the proof of Lemma 2.1 we obtain

$$\Big|\frac{it-1}{t}\sum_{m=0}^{n}(-1)^n\frac{(n+m)!}{m!(n-m)!}\frac{i^m}{(2t)^m}\Big| \le \frac{\sqrt{t^2+1}}{t}e. \tag{2.6}$$

For the second sum on the right side of (2.5) we have

$$\Big|\sum_{m=1}^{n}(-1)^n\frac{(n+m)!}{m!(n-m)!}\frac{i^m}{(2t)^m}\frac{m}{t}\Big| \le$$

$$\sum_{m=1}^{n}\frac{(n-m)!}{(n-m)!}\frac{1}{(m-1)!}\frac{(n-m+1)\dots n(n+1)\dots(n+m)}{n^m(2n)^m}\frac{1}{t} < \frac{e}{t}, \tag{2.7}$$

where we used the assumption that $n^2 < t$ and again followed the argument in Lemma 2.1.

From (2.5) by the triangle inequality with use of (2.6) and (2.7) we yield

$$|\partial_t h_n^{(1)}(t)| < \frac{\sqrt{2}}{\sqrt{\pi}}\Big(\frac{\sqrt{t^2+1}}{t^2}e + \frac{1}{t^2}e\Big)$$

and complete the proof of (2.3). □

LEMMA 2.4. *If* $0 < t$, *then*

$$|\partial_t h_n^{(1)}(t)| \le \frac{\sqrt{2}}{\sqrt{\pi}t}\Big(\frac{\sqrt{t^2+1}}{t} + \frac{n}{t}\Big)\Big(1+\frac{n}{t}\Big)^n. \tag{2.8}$$

PROOF. As in the proof of Lemma 2.3 we will bound two terms in (2.5). We have

$$\Big|\frac{it-1}{t}\sum_{m=0}^{n}(-1)^n\frac{(n+m)!}{m!(n-m)!}\frac{i^m}{(2t)^m}\Big| \le \frac{\sqrt{t^2+1}}{t}\Big(1+\frac{n}{t}\Big)^n, \tag{2.9}$$

by repeating the proof of Lemma 2.2.

For the second sum on the right side of (2.5) by the triangle inequality we have

$$\Big|\sum_{m=1}^{n}(-1)^n\frac{(n+m)!}{m!(n-m)!}\frac{i^m}{(2t)^m}\frac{m}{t}\Big| \le$$

$$\frac{1}{t}\sum_{m=1}^{n}\frac{n!}{m!(n-m)!}(n+1)\dots(n+m)\frac{n}{(2t)^m} = \frac{n}{t}\Big(1+\frac{n}{t}\Big)^n, \tag{2.10}$$

where we again followed the argument in Lemma 2.2.

Combining (2.5), (2.9), and (2.10) we yield

$$|\partial_t h_n^{(1)}(t)| \le \frac{\sqrt{2}}{\sqrt{\pi}t}(\frac{\sqrt{t^2+1}}{t}(1+\frac{n}{t})^n + \frac{n}{t}(1+\frac{n}{t})^n),$$

and complete the proof of (2.8). □

3. Proof of main results

For a (L^2-) function u on the sphere ∂B_R we have the orthonormal expansion

$$u(x) = \sum_{n=0}^{\infty} u_n Y_n(\sigma; u)$$

and introduce the low frequency projector

$$P_N u(x) = \sum_{n=0}^{N} u_n Y_n(\sigma; u).$$

LEMMA 3.1. *We have the following stability estimate:*

$$\|P_N u\|_{(0)}(\partial B_R) \le \frac{\sqrt{2}}{\sqrt{\pi}} e\varepsilon_1. \tag{3.1}$$

This result follows from (2.2) and (1.5). It shows Lipschitz stability of the low frequency part $P_N u$ from low frequency part of A. Since we choose $N = [kR]$, this part well approximates u when k is large.

Now we give a proof of Theorem 1.1

PROOF. Using the representation (1.4) we yield

$$\|u\|^2_{(0)}(\partial B_R) = \int_{\partial B_R} |u|^2(x) d\Gamma(x) =$$

$$k^2 \int_{\partial B_R} |\sum_{n=0}^{\infty} i^n a_n h_n^{(1)}(kR) Y_n(\sigma)|^2 d\Gamma(x) =$$

$$k^2 R^2 \sum_{n=0}^{\infty} |a_n|^2 |h_n^{(1)}(kR)|^2,$$

due to orthonormality of the system Y_n on the unit sphere. We let $N_1 = [\sqrt{E+k}]$ and consider two cases: 1) $N+1 \le N_1$ and 2) $N_1 \le N$.

In case 1) we split the last sum into three terms obtaining

$$\|u\|^2_{(0)}(\partial B_R) = k^2 R^2 (\sum_{n=0}^{N} |a_n|^2 |h_n^{(1)}(kR)|^2 +$$

$$\sum_{n=N+1}^{N_1} |a_n|^2 |h_n^{(1)}(kR)|^2 + \sum_{n=N_1+1}^{\infty} |a_n|^2 |h_n^{(1)}(kR)|^2). \tag{3.2}$$

We have

$$(1+\frac{N_1}{kR})^{2N_1}\varepsilon_2^2 = e^{2N_1 log(1+\frac{N_1}{kR})-2E} \le e^{2\frac{N_1^2}{kR}-2E} \le$$

$$e^{2\frac{E+k}{kR}-2E} \le e^{\frac{2}{R}-E} = e^{\frac{2}{R}}\varepsilon_2, \tag{3.3}$$

where we used that $log(1+x) < x$, when $0 < x$, that $N_1^2 \le E+k$, and that $2 \le kR$.

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Observe that

$$k^2R^2\sum_{n=N_1+1}^{\infty}|a_n|^2|h_n^{(1)}(kR)|^2\leq$$

$$\frac{1}{(N_1+1)^2}k^2R^2\sum_{n=N_1+1}^{\infty}n^2|a_n|^2|h_n^{(1)}(kR)|^2\leq R^2\frac{M_1^2}{(N_1+1)^2} \tag{3.4}$$

due to (1.5), (1.4).

Finally from (3.2) by using (2.2), (2.3),(3.3), and (3.4) we obtain

$$\|u\|^2_{(0)}(\partial B_R)\leq$$

$$k^2R^2\frac{2e^2}{\pi(kR)^2}\varepsilon_1^2+k^2R^2e^{\frac{2}{R}}\frac{2}{\pi k^2R^2}\varepsilon_2+R^2\frac{M_1^2}{(N_1+1)^2}$$

which gives (1.6) because of the choice of N_1.

In case 2) instead of (3.2) we write

$$\|u\|^2_{(0)}(\partial B_R)=$$

$$k^2R^2(\sum_{n=0}^{N}|a_n|^2|h_n^{(1)}(kR)|^2+\sum_{n=N+1}^{\infty}|a_n|^2|h_n^{(1)}(kR)|^2). \tag{3.5}$$

As in (3.4) we have

$$k^2\sum_{n=N+1}^{\infty}|a_n|^2|h_n^{(1)}(kR)|^2\leq\frac{M_1^2}{(N+1)^2}. \tag{3.6}$$

Similarly to case 1), from (3.5) by using (2.1) and (3.6) we yield

$$\|u\|^2_{(0)}(\partial B_R)\leq k^2R^2\frac{2e^2}{\pi(kR)^2}\varepsilon_1^2+R^2\frac{M_1^2}{(N+1)^2}\leq$$

$$\frac{2e^2}{\pi}\varepsilon_1^2+R^2\frac{M_1^2}{(N_1+1)^2}\leq\frac{2e^2}{\pi}\varepsilon_1^2+R^2\frac{M_1^2}{E+k},$$

because in case 2) $N_1\leq N$ and $E+k\leq(N_1+1)^2$. So again (1.6) follows.

Now we will prove (1.7).

We consider the same two cases: 1) $N+1\leq N_1$ and 2) $N_1\leq N$.

In case 1), as in the previous proof, we have the equality (3.2). Now we bound the second term on its right side in a different way:

$$k^2R^2\sum_{n=N+1}^{N_1}|a_n|^2|h_n^{(1)}(kR)|^2=\sum_{n=N+1}^{N_1}\frac{kR}{n}|a_n||h_n^{(1)}(kR)|kRn|a_n||h_n^{(1)}(kR)|\leq$$

$$R(\sum_{n=N+1}^{N_1}\frac{k^2R^2}{n^2}|a_n|^2|h_n^{(1)}(kR)|^2)^{\frac{1}{2}}(\sum_{n=N+1}^{N_1}k^2n^2|a_n|^2|h_n^{(1)}|(kR)^2)^{\frac{1}{2}}, \tag{3.7}$$

when we use the Cauchy-Schwarz inequality. Bounding the first term on the right side of (3.7) via (2.3) and the second term from the definition (1.5) of the Sobolev

norm and (1.4) we yield

$$k^2R^2\sum_{n=N+1}^{N_1}|a_n|^2|h_n^{(1)}(kR)|^2\le$$

$$\frac{\sqrt{2}}{\sqrt{\pi}(N+1)}(1+\frac{N_1}{kR})^{N_1}R(\sum_{n=N+1}^{N_1}|a_n|^2)^{\frac12}M_1=$$

$$\frac{\sqrt{2}R}{\sqrt{\pi}(N+1)}(1+\frac{N_1}{kR})^{N_1}R\varepsilon_2M_1\le\sqrt{\frac{2}{\pi}}R\frac{1}{\sqrt{kR}}e^{\frac1R}M_1\varepsilon_2^{\frac12}, \tag{3.8}$$

where we used (3.3).

From (3.2) by using (3.8) we derive that

$$\|u\|^2_{(0)}(\partial B_R)\le$$

$$k^2R^2\frac{2e^2}{\pi(kR)^2}\varepsilon_1^2+\sqrt{\frac{2R}{\pi}}\frac{1}{\sqrt{k}}e^{\frac1R}M_1\varepsilon_2^{\frac12}+R^2\frac{M_1^2}{(N_1+1)^2},$$

which as above produces (1.7).

Case 2) is considered exactly as in the proof of (1.6). □

Now we similarly prove Theorem 1.2.

Proof. Now we choose $N_1=[\sqrt{E+k}]-1$ and again consider two cases: 1) $N+1\le N_1$ and 2) $N_1\le N$.

From (1.3) using $t=kr$ we obtain

$$\partial_ru(x)=ik^2\sum_{n=0}^{\infty}a_n\partial_th_n^{(1)}(kr)Y_n(\sigma,A). \tag{3.9}$$

In case 1) similarly to (3.2) from (3.9) we have

$$\|\partial_ru\|^2_{(0)}(\partial B_R)=k^4R^2(\sum_{n=0}^{N}|a_n|^2|\partial_th_n^{(1)}(kR)|^2+$$

$$\sum_{n=N+1}^{N_1}|a_n|^2|\partial_th_n^{(1)}(kR)|^2+\sum_{n=N_1+1}^{\infty}|a_n|^2|\partial_th_n^{(1)}(kR)|^2). \tag{3.10}$$

Using Lemma 2.4 and the obvious inequality $\frac{t^2+1}{t^2}\le\frac54$, provided $2\le t$, we obtain

$$|\partial_th_n^{(1)}(kR)|^2\le\frac{2}{\pi k^2R^2}\frac54(1+\frac{n}{kR})^{2(n+1)}\le\frac{1}{k^2R^2}(1+\frac{n}{kR})^{2(n+1)}.$$

Similarly to (3.3),

$$(1+\frac{N_1}{kR})^{2(N_1+1)}\varepsilon_2^2\le e^{2\frac{N_1(N_1+1)}{kR}-2E}\le$$

$$e^{2\frac{(N_1+1)^2}{kR}-2E}\le e^{-E+\frac2R}=e^{\frac2R}\varepsilon_2, \tag{3.11}$$

because $N_1=[\sqrt{E+k}]-1$. As in (3.4), by using (3.9),(1.5), we obtain

$$k^4R^2\sum_{n=N_1+1}^{\infty}|a_n|^2|\partial_th_n^{(1)}(kR)|^2\le R^2\frac{M_2^2}{(N_1+1)^2}.$$

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Hence from (3.10), (2.4) by using that $\frac{\sqrt{t^2+1}+1}{t} \leq \frac{\sqrt{5}+1}{2}$ when $2 \leq t$ we obtain

$$\|\partial_r u\|^2_{(0)}(\partial B_R) \leq \frac{2e^2}{\pi}(\frac{\sqrt{5}+1}{2})^2 k^2 \varepsilon_1^2 + e^{\frac{2}{R}} k^2 \varepsilon_2 + R^2 \frac{M_2^2}{(N_1+1)^2}$$

Case 2) is considered exactly as in Theorem 1.1 by splitting into two terms instead of three in (3.10).

Now (1.8) follows because $\sqrt{E+K} - 1 \leq N_1 + 1$. □

4. Application to linearized inverse obstacle scattering

We consider a solution u_0 of the simplest scattering problem

$$\Delta u_0 + k^2 u_0 = 0 \text{ in } \mathbb{R}^3 \setminus \bar{D}_0, \tag{4.1}$$

with the Dirichlet boundary condition (soft obstacle)

$$u_0 = 1 \text{ on } \partial D_0 \tag{4.2}$$

and with the Sommerfeld radiation condition (1.2) for u_0. Here D_0 is a bounded domain with C^2-boundary and with connected complement of $\bar{D}$.

More important in applications is the hard obstacle problem where the Dirichlet boundary condition (4.2) is replaced with the Neumann condition

$$\partial_\nu u_1 = 1 \text{ on } \partial D_0 \tag{4.3}$$

(ν is the exterior unit normal) for the solution u_1 to the Helmholtz equation (4.1) with the radiation condition (1.2).

We will consider obstacle $D_0 = B_R$ in $\mathbb{R}^3$. Then the scattering problem (4.1), (4.2) has the explicit solution

$$u_0(x) = \frac{R}{e^{ikR}} \frac{e^{ikr}}{r}. \tag{4.4}$$

and the hard scattering problem has the solution

$$u_1(x) = \frac{R^2}{(ikR-1)e^{ikR}} \frac{e^{ikr}}{r}. \tag{4.5}$$

Observe that u_0, u_1 can be viewed as incident spherical waves.

Let $D = \{x : r < R + d(\sigma)\}$ where d is a function on ∂B_1 with small norm in C^2. It is known [**H**] that the solution u to the scattering problem (4.1), (4.2) with D_0 replaced by D is $u_0 + v_0 + \dots$ with the scattering amplitude $A_0 + A(v_0) + \dots$ where A_0 is the scattering amplitude of u_0, $A(v_0)$ is the scattering amplitude of the solution v_0 to the following scattering problem

$$\Delta v_0 + k^2 v_0 = 0 \text{ in } \mathbb{R}^3 \setminus \bar{D}_0, \tag{4.6}$$

$$v_0 = -d\partial_r u_0 \text{ on } \partial D_0 \tag{4.7}$$

with the Sommerfeld condition (1.2) for v_0. The term $\dots$ has the norm bounded by $C\|d\|_0^2$.

The linearized hard obstacle problem is similarly the following scattering problem

$$\Delta v_1 + k^2 v_1 = 0 \text{ in } \mathbb{R}^3 \setminus \bar{D}_0, \tag{4.8}$$

$$\partial_r v_1 = k^2 u_1 d \text{ on } \partial D_0 \tag{4.9}$$

with the Sommerfeld condition (1.2) for v_1.

Unique solvalibity of the direct scattering problems in Sobolev and Hölder spaces is well known [**CK**], [**I**], [**T**]. For example, for any $d \in H^1(\partial D_0)$ there is an unique radiating solution $v_0 \in H^1(B_\rho \setminus \bar B_R)$ (for any $\rho > R$) to the linearized direct scattering problem (4.6), (4.7).

The linearized inverse obstacle scattering problem is to find D (or, equivalently, d) from $A(v_0)$ or $A(v_1)$.

COROLLARY 4.1. *For a solution d of the inverse soft obstacle problem we have*

$$\|d\|^2_{(0)}(\partial B_R) \le \frac{R^2}{k^2R^2+1}(\frac{2e^2}{\pi}\varepsilon_1^2 + \frac{2}{\pi}e^{\frac{2}{R}}\varepsilon_2) + R^2\frac{\|d\|^2_{(1)}(\partial B_R)}{E+k}$$

and

$$\|d\|^2_{(0)}(\partial B_R) \le$$

$$\frac{R^2}{k^2R^2+1}(\frac{2e^2}{\pi}\varepsilon_1^2 + \sqrt{\frac{2(k^2R^2+1)}{\pi kR}}e^{\frac{1}{R}}\|d\|_{(1)}(\partial B_R)\varepsilon_2^{\frac12}) + R^2\frac{\|d\|^2_{(1)}(\partial B_R)}{E+k},$$

where $\varepsilon_1, \varepsilon_2, E$ are defined in Theorem 1.1 with A is replaced by $A(v_0)$.

PROOF. From (4.4) by elementary calculations

$$\partial_r u_0(R\sigma) = \frac{R}{e^{ikR}}\frac{ike^{ikR}R - e^{ikR}}{R^2} = \frac{ikR-1}{R}$$

Hence $|\partial_r u_0|^2 = \frac{k^2R^2+1}{R^2}$ and

$$\|v_0\|^2_{(1)}(\partial B_R) = \frac{k^2R^2+1}{R^2}\|d\|^2_{(1)}(\partial B_R).$$

So this Corollary follows from (4.7) and Theorem 1.1. □

COROLLARY 4.2. *For a solution d of the inverse hard obstacle problem we have*

$$\|d\|^2_{(0)}(\partial B_R) \le$$

$$\frac{k^2R^2+1}{k^2R^2}(\frac{e^2}{\pi}(3+\sqrt5)\varepsilon_1^2 + e^{\frac{2}{R}}\varepsilon_2 + R^2\frac{\|d\|^2_{(1)}(\partial B_R)}{E+k-2\sqrt{E+k}+1},$$

where $\varepsilon_1, \varepsilon_2, E$ are defined in Theorem 1.2 with A is replaced by $A(v_1)$.

PROOF. Observe that, according to (4.5), (4.9),

$$\|\partial_r v_1\|^2_{(1)}(\partial B_R) = k^4\frac{R^2}{k^2R^2+1}\|d\|^2_{(1)}(\partial B_R).$$

Now from (4.9), (4.5) and Theorem 1.2 we have

$$\|d\|^2_{(0)}(\partial B_R) = \frac{1}{k^4}\frac{1}{|u_1|^2}\|\partial_r v_1\|^2_{(0)}(\partial B_R) \le$$

$$\frac{1}{k^2}\frac{k^2R^2+1}{k^2R^2}(\frac{e^2}{\pi}(3+\sqrt5)k^2\varepsilon_1^2 + e^{\frac{2}{R}}k^2\varepsilon_2) + R^2\frac{\|d\|^2_{(1)}(\partial B_R)}{E+k-2\sqrt{E+k}+1},$$

and Corollary 4.2 follows. □

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5. Conclusion

We think that increasing stability is an important feature which leads to higher resolution of numerical algorithms. It is important to collect numerical evidence of this phenomenon. We tried to obtain most explicit forms of stability estimates to make them useful in particular for numerical solution of inverse scattering problems.

It is interesting to expand Lipschitz stability zone: i.e. to replace the condition $n^2 < t$ of Lemma 2.1 by the most natural condition $n < \theta k$ with some $\theta < 1$. Given numerous previous efforts, this seems to be a hard problem. The results of this paper most likely imply similar increasing stability estimates when $B(0, R)$ is replaced by a strictly convex domain D. Indeed, one can represent the complement of such D as the union of the family of the exteriors of spheres whose radii and centers are contained in a bounded set and use bounds (1.6), (1.7) for these spheres. For general convex obstacles we do not expect such explicit and simple bounds.

Much more challenging is to show increasing stability for soft and hard (convex) obstacles. It is not clear even how to handle linearized problems near a sphere when the incident wave is traditional $e^{ik\xi\cdot x}$ with $|\xi| = 1$. While the solution u_0 of the unperturbed soft scattering problem is well known [**CK**], [**T**], its is difficult to control zeros of its normal derivative on the boundary and hence to use (4.7).

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Inverse scattering on multi-dimensional asymptotically hyperbolic orbifolds

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Dedicated to James Ralston on the occasion of his 70th birthday

Abstract. We study the inverse scattering associated with n-dimensional asymptotically hyperbolic orbifolds ($n \geq 2$) having a finite number of cusps and regular ends. We introduce a generalized S-matrix by observing the Fourier coefficients of solutions of the Helmholtz equation at a cusp, and show that it determines the manifolds with its Riemannian metric and the orbifold structure.

1. Introduction

1.1. Assumptions on the orbifold. We consider an n-dimensional ($n \geq 2$) connected Riemannian orbifold $\mathcal{M}$, which is written as a union of open sets:

$$\mathcal{M} = \mathcal{K} \cup \mathcal{M}_1 \cup \cdots \cup \mathcal{M}_{N+N'}, \tag{1}$$

where $N \geq 1, N' \geq 0$ are integers and $\mathcal{M}_i \cap \mathcal{M}_j = \emptyset$ if $i \neq j$. A part $\mathcal{M}_i$ is henceforth called *an end*. The following assumptions are imposed on $\mathcal{M}$.

(A-1) *$\mathcal{K}$ is a relatively compact n-dimensional orbifold.*

(A-2) *Letting $\approx$ stand for "diffeomorphic", we have*

$$\mathcal{M}_j \approx \begin{cases} M_j \times (1, \infty), & for \quad 1 \leq j \leq N, \\ M_j \times (0, 1), & for \quad N+1 \leq j \leq N+N', \end{cases}$$

where, in both cases, M_j is a compact $(n-1)$-dimensional Riemannian orbifold whose metric is denoted by $h_j(x, dx)$.

(A-3) *If $x \in M_j^{sing}$, see (9) for M^{sing}, it has a neighbourhood U_x such that for $1 \leq j \leq N$, $U_x \times (1, \infty)$ has a uniformizing cover, and for $N+1 \leq j \leq N+N'$, $U_x \times (0, 1)$ has a uniformizing cover. Namely, there is an open set $\widetilde{U}_x \subset R^{(n-1)}$, $0 \in \widetilde{U}_x$ and a discrete subgroup $G_x \subset SO(n-1)$ acting on $\widetilde{U}_x$. Denoting by π the corresponding surjection $\pi : \widetilde{U}_x \times (1, \infty) \to U_x \times (1, \infty)$ with $U_x = \widetilde{U}_x / G_x$, there is a metric $\widetilde{g}$ in*

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$\widetilde{U}_x$ such that $\pi^* g = \widetilde{g}$ and

$$d\widetilde{s}^2 = \widetilde{g}(\widetilde{x}, y, d\widetilde{x}, dy) = \frac{(dy)^2 + \widetilde{h}_j(\widetilde{x}, y, d\widetilde{x}, dy)}{y^2}, \tag{2}$$

$$\widetilde{x} \in \widetilde{U}_x, \quad y \in \begin{cases} (1, \infty), & 1 \le j \le N, \\ (0, 1), & N+1 \le j \le N+N'. \end{cases}$$

Here the length element $\widetilde{h}_j(\widetilde{x}, y, d\widetilde{x}, dy)$ has the form:
(i) For $1 \le j \le N$,

$$\widetilde{h}_j(\widetilde{x}, y, d\widetilde{x}, dy) = \widetilde{h}_j(\widetilde{x}, d\widetilde{x}). \tag{3}$$

(ii) For $N+1 \le j \le N+N'$,

$$\begin{aligned} &\widetilde{h}_j(\widetilde{x}, y, d\widetilde{x}, dy) \\ &= \widetilde{h}_j(\widetilde{x}, d\widetilde{x}) + \sum_{p,q=1}^{n-1} a_{j,pq}(\widetilde{x}, y) d\widetilde{x}_p d\widetilde{x}_q + \sum_{p=1}^{n-1} b_{j,p}(\widetilde{x}, y) d\widetilde{x}_p dy + c_j(\widetilde{x}, y) dy^2. \end{aligned} \tag{4}$$

Here, $a = a_{j,pq}, b_{j,p}, c_j$ satisfy, for any α, β,

$$|(\partial_{\widetilde{x}})^\alpha (y\partial_y)^\beta a(\widetilde{x}, y)| \le C_{\alpha\beta} (1 + |\log y|)^{-\min(|\alpha|+\beta, 1) - 1 - \epsilon_0}, \tag{5}$$

for some constant $\epsilon_0 > 0$. Moreover,

$$\gamma^* \widetilde{g} = \widetilde{g}, \quad \text{for} \quad \gamma \in G_x.$$

If $x \in M^{reg} = M \setminus M^{sing}$, it has a neighborhood U_x for which there is a diffeomorphism $\pi : \widetilde{U}_x \to U_x$ such that $\widetilde{\pi}^* g$ has the form (2) and satisfies i and (ii.

We give a precise definition of an orbifold in Subsection 1.4. The orbifold at infinity, M_j, is called *a cusp* for $1 \le j \le N$ and *a regular infinity* for $N+1 \le j \le N+N'$. Sometimes $\mathcal{M}_j$ is called a cusp if M_j is a cusp. We also call $\mathcal{M}_j$ *regular end* if M_j is a regular infinity. Let $H = -\Delta_g - (n-1)^2/4$, where Δ_g is the Laplace-Beltrami operator for $\mathcal{M}$. It has continuous spectrum $\sigma_c(H) = [0, \infty)$, and the discrete spectrum $\sigma_d(H) \subset (-\infty, 0)$. If $N' = 0$, H may have embedded eigenvalues in $(0, \infty)$, which are discrete with possible accumulation points 0 and ∞.

The above assumptions allow important classes of hyperbolic orbifolds $G \backslash \mathbf{H}^n$, where $\mathbf{H}^n$ is the n-dimensional hyperbolic space and G is a discrete subgroup of isometries on $\mathbf{H}^n$. If $n = 2$, all fundamental domains obtained by geometrically finite Fuchsian groups satisfy the assumption (A-1), (A-2), (A-3), where each M_j is a C^∞ manifold, in fact, S^1. For example, the modular surface $SL(2, \mathbf{Z}) \backslash H^2$ is a well-known example of 2-dimensional orbifold with cusp, see e.g. [**23**] for general considerations or [**14**] for results related to the present paper. We also give a 3-dimensional example in §2 by taking $G = SL(2, \mathbf{Z} + i\mathbf{Z})$, in which case $N' = 0$, and all M_j's are not C^∞ manifolds but orbifolds with singularities.

1.2. Inverse scattering from regular ends. When $\mathcal{M}$ is a smooth Riemannian manifold (not orbifold) having only regular ends, one can introduce the (physical) *S-matrix* by observing the behavior of solutions to the time-dependent Schrödinger equation or the wave equation on $\mathcal{M}$. An equivalent way is to observe the asymptotic expansion of solutions to the Helmholtz equation on $\mathcal{M}$ in the function space $\mathcal{B}^*$, first introduced in [**1**] for Euclidian case. Roughly, $u \in \mathcal{B}^*$ means that u behaves like $O(y^{(n-1)/2})$ on each end. One can then talk

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about the inverse problem. Suppose we are given two such manifolds $\mathcal{M}^{(1)}$, $\mathcal{M}^{(2)}$ with $\mathcal{M}^{(i)}_{N_i+N_i'}$ being regular ends for $i = 1, 2$. Assume also that we are given, for all $k > 0$, the component $\widehat{S}^{(i)}_{N_i+N_i' N_i+N_i'}(k)$ of the S-matrix, which describes the wave coming in through $\mathcal{M}^{(i)}_{N_i+N_i'}$ and going out of $\mathcal{M}^{(i)}_{N_i+N_i'}$. Suppose that $\widehat{S}^{(1)}_{N_1+N_1' N_1+N_1'}(k) = \widehat{S}^{(2)}_{N_2+N_2' N_2+N_2'}(k)$ for all $k > 0$. If, furthermore, two ends $\mathcal{M}^{(1)}_{N_1+N_1'}$ and $\mathcal{M}^{(2)}_{N_2+N_2'}$ are known to be isometric, these two manifolds $\mathcal{M}^{(1)}$ and $\mathcal{M}^{(2)}$ are shown to be isometric (see [**13**], where more general results are discussed).

Sa Barreto [**30**] proved that, under the framework of scattering theory due to Melrose [**27**], two such manifolds are isometric, if the whole scattering matrix for all energies coincide, without assuming that one end is known to be isometric. In Melrose's theory of scattering metric, $(ds)^2$ is assumed to have an asymptotic expansion with respect to y around $y = 0$ (which roughly corresponds to the estimate 5), with $O(y)$, $y \to 0$, in the right-hand side.

1.3. Main result. The problem we address in this paper is the case in which we observe the waves coming in and going out from a cusp. Recall that the end $\mathcal{M}_1$ has a cusp at infinity.

Since the continuous spectrum due to the presence of the cusp is simple, the associated S-matrix component $\widehat{S}_{11}(k)$ is a complex number, and it does not have enough information to determine the whole orbifold (see Zelditch [**33**]). Therefore we generalize the notion of S-matrix in the following way.

The Helmholtz equation has the following form in the cusp $\mathcal{M}_1$:

$$\left[-y^2(\partial_y^2 + \Delta_h) + (n-2)y\partial_y - \frac{(n-1)^2}{4}\right] u = k^2 u, \tag{6}$$

where $k > 0$ and Δ_h is the Laplace-Beltrami operator for M_1. Let $\lambda_0 \le \lambda_1 \le \cdots$ be the eigenvalues of $-\Delta_h$ and $\varphi_0, \varphi_1, \cdots$ be the associated orthnormal eigenfunctions. Then, on the end $\mathcal{M}_1$, any solution of the equation (6) is represented as

$$\begin{aligned} u = {} & a_0 y^{(n-1)/2-ik} + \sum_{m=1}^{\infty} a_m y^{(n-1)/2} I_{-ik}(\sqrt{\lambda_m} y)\varphi_m(x) \\ & + b_0 y^{(n-1)/2+ik} + \sum_{m=1}^{\infty} b_m y^{(n-1)/2} K_{ik}(\sqrt{\lambda_m} y)\varphi_m(x), \end{aligned} \tag{7}$$

where $I_\nu(z), K_\nu(z)$ are modified Bessel functions. Recall that $I_\nu(z)$ is exponentially growing and $K_\nu(z)$ is exponentially decreasing as $z \to \infty$. We call the operator

$$\mathcal{S}_{11}(k) : \{a_n\} \to \{b_n\} \tag{8}$$

the (11)−component of the *generalized S-matrix*, see §4 for the precise definition. We shall show that $\mathcal{S}_{11}(k)$, $k > 0$ determines the whole orbifold $\mathcal{M}$.

Our main result is the following.

THEOREM 1.1. *Suppose two Riemannian orbifolds $\mathcal{M}^{(1)}$ and $\mathcal{M}^{(2)}$ satify the assumptions (A-1), (A-2), (A-3). Assume that the (11) components of the generalized scattering matrix coincide :*

$$\mathcal{S}^{(1)}_{11}(k) = \mathcal{S}^{(2)}_{11}(k), \quad \forall k > 0, \quad k^2 \notin \sigma_p(H^{(1)}) \cup \sigma_p(H^{(2)}).$$

Assume also that the ends $\mathcal{M}_1^{(1)}$ and $\mathcal{M}_1^{(2)}$ are isometric. Then $\mathcal{M}^{(1)}$ and $\mathcal{M}^{(2)}$ are isometric orbifolds.

The main Theorem 1.1 roughly means that we send exponentially growing waves into $\mathcal{M}$ from the cusp $\mathcal{M}_1$ and observe the exponentially decaying waves in the same end. Then, if the resulting observations coincide for two asymptotically hyperbolic orbifolds, then these two orbifolds are isometric. Let us also remark that the number of ends are not assumed to be equal a priori.

The principle idea of the proof of this theorem is to introduce some artificial boundaries in $\mathcal{M}_1^i$, $i = 1, 2$, which cut off $\mathcal{M}_{int}^i = \mathcal{K}^i \cup \mathcal{M}_2^i \cup \cdots \cup \mathcal{M}_{l_i}^i$, to show that the Neumann-to-Dirichlet maps associated with $\mathcal{M}_{int}^i$ coincide on these boundaries and then to apply the boundary control (BC) method to the resulting Gel'fand problem. In this paper, we explain the basic notions and the outline of the proof of the main theorem. The details can be found in [**15**].

Let us also note that in recent years spectral, scattering and inverse scattering for asymptotically hyperbolic manifolds has been atracting much interest, see e.g. [**5**], [**9**], [**10**], [**11**], [**12**], [**28**], [**32**].

1.4. Riemannian orbifolds. Here we recall basic notions of orbifolds, see [**29**, **31**] for further details. A complete metric space $(\mathcal{M}, d)$ is called a *Riemannian orbifold* of dimension n if, for any $p \in \mathcal{M}$,

(i) There exists $r = r(p) > 0$, a domain $\tilde{U}_p = \widetilde{B}_r \subset \mathbf{R}^n$ which is a ball with respect to a Riemannian metric $\widetilde{g}_p$ centered at 0 and a finite group $G_p \subset SO(n)$ acting by isometries on $\widetilde{B}_r$.

(ii) For all $\gamma \in G_p$ it holds that $\gamma \cdot 0 = 0$ and the action of G_p on $\widetilde{B}_r$ is faithful.

(iii) For the metric ball $U_p = B_r(p) \subset \mathcal{M}$ there exists a continuous surjection $\pi_p : \widetilde{B}_r \to B_r(p)$ such that $\pi_p(0) = p$, moreover for $\tilde{x} \in \widetilde{B}_r$ and $x = \pi_p(\tilde{x})$ it holds $\pi_p^{-1}(x) = \{\gamma \cdot \tilde{x}\,;\ \gamma \in G_p\}$.

(iv) For all $x, y \in B_r(p)$ the distance $d(x, y)$ satisfies $d(x, y) = \min\{\tilde{d}(\tilde{x}, \tilde{y})\,;\ \tilde{x} \in \pi_p^{-1}(x),\ \tilde{y} \in \pi_p^{-1}(y)\}$, where $\tilde{d}$ is the distance function on $\widetilde{B}_r$ with respect to the metric $\widetilde{g}_p$.

We say that the Riemannian ball $\widetilde{U}_p = \widetilde{B}_r$ with the Riemannian metric $\widetilde{g}_p$ is the uniformizing cover of U_p.

We denote

$$\mathcal{M}_{sing} = \{p \in \mathcal{M}\,;\, G_p \neq \{1\}\}, \quad \mathcal{M}_{reg} = \mathcal{M} \setminus \mathcal{M}_{sing}. \tag{9}$$

The elements in $\mathcal{M}_{sing}$ are called *singular points* of $\mathcal{M}$. Then,

(RO-1) *$\mathcal{M}_{sing}$ is a closed subset of $\mathcal{M}$.*

(RO-2) *For each $p \in \mathcal{M}$, $\gamma \in G_p$, $\pi_p \circ \gamma = \pi_p$ on $\widetilde{U}_p$.*

(RO-3) *If $p \in M_{reg}$, π_p is a homeomorphism from $\widetilde{U}_p$ to U_p.*

(RO-4) *Let $U_p \cap U_q \neq \emptyset$ for $p, q \in \mathcal{M}$, for any $\widetilde{x} \in \widetilde{U}_p$ and $\widetilde{y} \in \widetilde{U}_q$ such that $\pi_p(\widetilde{x}) = \pi_q(\widetilde{y})$, there are neighborhoods $\widetilde{x} \in V_{\widetilde{x}} \subset \widetilde{U}_p$, $\widetilde{y} \in V_{\widetilde{y}} \subset \widetilde{U}_q$ and a Riemannian isometry $\psi : V_{\widetilde{x}} \to V_{\widetilde{y}}$ such that $\psi(\widetilde{x}) = \widetilde{y}$.*

Two Riemannian orbifolds $\mathcal{M}$, $\mathcal{M}'$ are said to be *isometric* if they satisfy the following conditions:

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(I-1) *There exists a homeomorphism* $f : \mathcal{M} \to \mathcal{M}'$ *such that* $f(\mathcal{M}_{reg}) = \mathcal{M}'_{reg}$, $f(\mathcal{M}_{sing}) = \mathcal{M}'_{sing}$, *and* $f\big|_{\mathcal{M}_{reg}} : \mathcal{M}_{reg} \to \mathcal{M}'_{reg}$ *is a Riemannian isometry.*
(I-2) *Let* $p \in \mathcal{M}_{sing}$ *and* $p' = f(p) \in \mathcal{M}'_{sing}$. *Then, for some* $r > 0$, *the uniformizing cover* $\widetilde{U}_p$ *of* $B_r(p)$ *and the uniformizing cover* $\widetilde{U}_{p'}$ *of* $B'_r(p')$, *there exists a Riemannian isometry* $\widetilde{F}_p : \widetilde{U}_p \to \widetilde{U}_{p'}$ *such that*

$$f \circ \pi_p = \pi'_{f(p)} \circ \widetilde{F}_p \quad on \quad \widetilde{U}_p. \tag{10}$$

Moreover, there exists a group isomorphism $i_p : G_p \to G'_{p'}$ *such that, for all* $\gamma \in G_p$, *we have*

$$\widetilde{F}_p \circ \gamma = (i_p\gamma) \circ \widetilde{F}_p \quad on\ \widetilde{U}_p. \tag{11}$$

To introduce a functional calculus on Riemannian orbifolds, we use a uniformising cover. We put $\widetilde{U}_p = B_r(\widetilde{p}\,; \widetilde{g}_p)$ for brevity. First let us note that there is a 1 to 1 correspondence between a (one-valued) function f on U_p and a G_p-invariant function $\widetilde{f}$ on $\widetilde{U}_p$:

$$f(\pi_p(z)) = \widetilde{f}(z), \quad z \in \widetilde{U}_p; \quad f(x) = \widetilde{f}(\pi_p^{-1}(x)), \quad x \in U_p. \tag{12}$$

Note also that a function $\widetilde{f}$ on $\widetilde{U}_p$ is G_p-invariant if and only if there exists a function F defined on $\widetilde{U}_p$ such that

$$\widetilde{f}(z) = \frac{1}{\#(G_p)} \sum_{\gamma \in G_p} F(\gamma \cdot z), \quad z \in \widetilde{U}_p.$$

We say that $f \in C^\infty(U_p)$ if $\widetilde{f}$ in (12) satisfies $\widetilde{f} \in C^\infty(\widetilde{U}_p)$, and $f \in H^m(U_p) =$ the Sobolev space of order m, if $\widetilde{f} \in H^m(\widetilde{U}_p)$. Then we have : $f \in C_0^\infty(U_p)$ if and only if $\widetilde{f} \in C_0^\infty(\widetilde{U}_p)$. The integral of a function f over U_p is defined by

$$\int_{U_p} f dU_p = \frac{1}{\#(G_p)} \int_{\widetilde{U}_p} \widetilde{f} d\widetilde{U}_p, \tag{13}$$

where $d\widetilde{U}_p$ is the Riemannian volume element of $\widetilde{U}_p$.

If $\mathcal{M}$ is compact, the set of singular points is also compact. We can then construct an open covering of $\mathcal{M}$, $\bigcup_{i=1}^m V_i = \mathcal{M}$, such that each V_i is one of the above U_p. By using the partition of unity $\{\chi_i\}_{i=1}^m$ subordinate to this covering, we define the integral over $\mathcal{M}$ by

$$\int_{\mathcal{M}} f d\mathcal{M} = \sum_{i=1}^m \int_{V_i} \chi_i f dV_i.$$

When $\mathcal{M}$ is non-compact, the situation may be more complicated and one needs to modify the above arguments, which we omit here.

By shrinking $\widetilde{U}_p$, we can assume that each $\widetilde{U}_p$ is in one coordinate patch. Let $z = (z_1, \cdots, z_n)$ be the associated local coordinate on $\widetilde{U}_p$ and $\sum_{i,j=1}^n \widetilde{g}_{ij}(z) dz_i dz_j$ the G_p-invariant Riemannian metric on $\widetilde{U}_p$. Then, letting $x = \pi_p(z)$, the Laplace-Beltrami operator Δ_g for the orbifold $\mathcal{M}$ is written as

$$\Delta_g f(x) = \Big(\frac{1}{\sqrt{\widetilde{g}}} \sum_{i,j=1}^n \frac{\partial}{\partial z_i} \sqrt{\widetilde{g}} \widetilde{g}^{ij} \frac{\partial}{\partial z_j} \widetilde{f} \Big) \left(\pi_p^{-1}(x)\right), \quad \widetilde{g} = \det\left(\widetilde{g}_{ij}\right).$$

2. 3-dimensional hyperbolic orbifolds

2.1. Kleinian group. Let $\mathbf{H}^3 = \{(x_1, x_2, y)\,; y > 0\}$ be the upper half space model of the 3-dimensional hyperbolic space. Representing $\mathbf{H}^3$ by quarternions $(x_1, x_2, y) \longleftrightarrow x_1\mathbf{1} + x_2\mathbf{i} + y\mathbf{j}$, and identifying $x_1\mathbf{1} + x_2\mathbf{i}$ with $z = x_1 + ix_2 \in \mathbf{C}$, we have

$$x_1\mathbf{1} + x_2\mathbf{i} + y\mathbf{j} = \begin{pmatrix} z & y \\ -y & \overline{z} \end{pmatrix} =: \zeta = z + yj.$$

Then, $SL(2, \mathbf{C})$ gives rise to a group which acts isometrically on $\mathbf{H}^3$:

$$SL(2, \mathbf{C}) \times \mathbf{H}^3 \ni (\gamma, \zeta) \to \gamma \cdot \zeta := (a\zeta + b)(c\zeta + d)^{-1}, \quad \gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

The mapping : $\gamma \to \gamma\cdot$ is 2 to 1, giving rise to a group isomorphic to $PSL(2, \mathbf{C}) = SL(2, \mathbf{C})/\{\pm I\}$. A discrete subgroup G of $PSL(2, \mathbf{C})$ is called a *Kleinian group*.

2.2. Picard group. As an example, we consider the Picard group

$$G = PSL(2, \mathbf{Z}[i]) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix}\,;\, a, b, c, d \in \mathbf{Z}[i],\ ad - bc = 1 \right\}, \tag{14}$$

where $\mathbf{Z}[i] = \mathbf{Z} + i\mathbf{Z}$ is the ring of Gaussian integers. The fundamental domain $\mathcal{M}$ of G is

$$\mathcal{M} = G\backslash\mathbf{H}^3 = \left\{ z + yj\,;\, |\mathrm{Re}\, z| \le \frac{1}{2},\ 0 \le \mathrm{Im}\, z \le \frac{1}{2},\ |z|^2 + y^2 \ge 1 \right\},$$

see Fig. 1, where the boundary sides are properly identified. See for details [**7**], Proposition 3.9, and [**15**], §3.

Then, the singular points of $\mathcal{M}$ consists of 8 lines and 4 points, which are the intersections of corresponding singular lines. The isotropy groups of the lines are either $\mathbf{Z}_2$ or $\mathbf{Z}_3$, while the isotropy groups of the singular points are generated by the corresponding groups of intersecting lines.

2.3. Orbifold structure on $\mathcal{M}$. Each point $p \in \mathcal{M}$ has the uniformizing cover $\widetilde{U}_p = \widetilde{B}_{r_p}(\tilde{p}) \subset \mathbf{H}^3$, where now we take $\widetilde{p} = p \in \mathbf{H}^3$, with isotopy group discribed above. If $p \in \mathcal{M}^{reg}$, we take $r_p = \mathrm{dist}(p, \mathcal{M}^{sing})$. If p lies on a singular line, we take r_p to be the distance to the other singular lines. If p is a singular point, r_p is the distance to the other singular points.

If $U_p \cap U_q \neq \emptyset$ and $\pi_p(\zeta) = \pi_q(\zeta')$, we let V_ζ, $V_{\zeta'}$ be small balls centered at ζ, ζ', and define ψ as an isometry from V_ζ to $V_{\zeta'}$ such that $\psi(\zeta) = \zeta'$, the construction of which is evident.

2.4. Orbifold structure of the horizontal slice. Since the isotropy group of a singular line is a subgroup of rotations with respect to this line, then, for any $t > 1$, the horizontal slice $M_t = \mathcal{M} \cap \{y = t\}$ is a compact 2-dimensional orbifold with singular points $-1/2 + tj,\ -1/2 + i/2 + tj,\ tj,\ i/2 + tj$. Here the covering is a disc in $\mathbf{R}^2$ with the scaled Euclidean metric. Note that the orbifold structure of M_t is independent of t.

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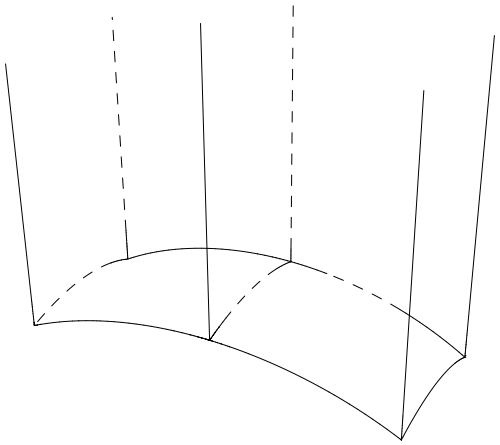

FIGURE 1. Fundamental domain for $PSL(2, \mathbf{Z}[i])$

3. Helmholtz equation and the S-matrix

Let $H = -\Delta_g - (n-1)^2/4$ be the shifted Laplacian on $\mathcal{M}$ with resolvent $R(z) = (H-z)^{-1}$. We introduce a Banach space $\mathcal{B}$ and its dual space $\mathcal{B}^*$ satisfying $\mathcal{B} \subset L^2(\mathcal{M}) \subset \mathcal{B}^*$ (see [**1**] for the Euclidean case). We state the definition of $\mathcal{B}^*$ omitting that of $\mathcal{B}$. Take a C^∞ partition of unity $\{\chi_j\}_{j=0}^{N+N'}$ on $\mathcal{M}$ such that for $j = 1, \cdots, N+N'$, $\operatorname{supp} \chi_j \subset \mathcal{M}_j$, $\chi_j(y) = 1$ for $y > 2$ and $j = 1, \cdots, N$, $\chi_j(y) = 1$ for $y < 1/2$, $j = N+1, \cdots, N+N'$. We put for a $L^2(M_j)$-valued function $u(y)$,

$$\|u\|^2_{\mathcal{B}^*,j} = \begin{cases} \sup\limits_{R>e} \dfrac{1}{\log R} \displaystyle\int_{2<y<R} \|u(y)\|^2_{L^2(M_j)} \frac{dy}{y^n}, & 1 \le j \le N, \\ \sup\limits_{R>e} \dfrac{1}{\log R} \displaystyle\int_{1/R<y<1/2} \|u(y)\|^2_{L^2(M_j)} \frac{dy}{y^n}, & N+1 \le j \le N+N'. \end{cases}$$

The $\|\cdot\|_{\mathcal{B}^*}$ norm is defined by

$$\|u\|_{\mathcal{B}^*} = \|\chi_0 u\|_{L^2(\mathcal{M})} + \sum_{j=1}^{N+N'} \|\chi_j u\|_{\mathcal{B}^*,j}.$$

One can then prove the following theorem.

THEOREM 3.1. *For $\lambda \in \sigma_e(H) \setminus \sigma_p(H)$, there exists a limit*

$$\lim_{\epsilon \to 0} R(\lambda \pm i\epsilon) \equiv R(\lambda \pm i0) \in \mathbf{B}(\mathcal{B}; \mathcal{B}^*)$$

in the weak $*$-sense. Moreover, for any compact interval $I \subset \sigma_e(H) \setminus \sigma_p(H)$, there exists a constant $C > 0$ such that

$$\|R(\lambda \pm i0) f\|_{\mathcal{B}^*} \le C \|f\|_{\mathcal{B}}, \quad \lambda \in I.$$

For $f, g \in \mathcal{B}$, $(R(\lambda \pm i0) f, g)$ is continuous with respect to $\lambda > 0$.

We prove this theorem by the classical method of integration by parts due to Eidus [**6**], which has been extended to the case of asymptotically hyperbolic manifolds in [**13**], Chapters 2 and 3. Note that [**13**] also deals with the case when the behavior of the coefficients is governed by (5). Although $\mathcal{M}$ has singularities because of the orbifold structure, these cause no extra difficulties if the computations used in [**13**] are carried out on a uniformizing cover $\widetilde{U}\times(1,\infty)$ or $\widetilde{U}\times(0,1)$ which are described in (A-3). In partucular, if M_j is a simple orbifold, $M_j = N_j/G_j$, then u satisfies the equation (6) and belongs to $\mathcal{B}^*(\mathcal{M}_j)$ if and only if $\widetilde{u}$ satisfies the equation (6) with $\widetilde{h}$ instead of h in $\mathcal{N}_j = N_j\times(1,\infty)$ or $\mathcal{N}_j = N_j\times(0,1)$ and belongs to $\mathcal{B}^*(\mathcal{N}_j)$. Here, $\widetilde{u}_j$ is the lift of u_j on $\mathcal{N}_j$ and $\widetilde{h}_j$ is defined by (3) or (4).

Using this theorem, one can construct a spectral representation for H. It is first defined, using the asymptotic expansion of the resolvent at infinity, as a bounded operator $\mathcal{F}_\pm(k)$ from $\mathcal{B}$ to $\mathbf{h}_\infty$, where

$$\mathbf{h}_\infty = \Big(\oplus_{i=1}^{N}\mathbf{C}\Big)\oplus\Big(\oplus_{i=N+1}^{N+N'}L^2(M_i)\Big). \tag{15}$$

Then, putting $(\mathcal{F}_\pm f)(k) = \mathcal{F}_\pm(k)f$ for $f\in\mathcal{B}$, $\mathcal{F}_\pm$ is extended as a unitary operator from the absolutely continuous subspace of H onto $L^2((0,\infty);\mathbf{h}_\infty;dk)$. Since $\mathcal{F}_\pm(k)Hf = k^2\mathcal{F}_\pm(k)f$, its adjoint $\mathcal{F}_\pm(k)^*\in\mathbf{B}(\mathbf{h}_\infty;\mathcal{B}^*)$ is an eigenoperator of H in the sense that

$$(H-k^2)\mathcal{F}_\pm(k)^*\psi = 0,\quad \psi\in\mathbf{h}_\infty.$$

One important role of this spectral representation is that it characterizes the space of solutions to the Helmholtz equation:

$$\mathcal{N}(k) := \{u\in\mathcal{B}^*\,;\,(H-k^2)u=0\} = \mathcal{F}_\pm(k)^*\mathbf{h}_\infty, \tag{16}$$

i.e. any u in $\mathcal{N}(k)$ can be written as a Poisson transform of an element of $\mathbf{h}_\infty$. This yields an asymptotic expansion of solutions to the Helmholtz equation. In the following theorem, $f\simeq g$ means that

$$\lim_{R\to\infty}\frac{1}{\log R}\int_{1/R<y<R}\|\chi_j(y)(f(y)-g(y))\|^2_{L^2(M_j)}\frac{dy}{y^n} = 0,\quad 1\le j\le N+N'.$$

THEOREM 3.2. *(1) For any $u\in\mathcal{N}(k)$, there exist unique $\psi^{(\pm)}\in\mathbf{h}_\infty$ such that*

$$\begin{aligned} u \simeq{}& \omega_-(k)\sum_{j=N+1}^{N+N'}\chi_j y^{(n-1)/2+ik}\psi_j^{(-)} + \omega_-^{(c)}(k)\sum_{j=1}^{N}\chi_j y^{(n-1)/2-ik}\widehat{\psi}_{j0}^{(-)}\\ &-\omega_+(k)\sum_{j=N+1}^{N+N'}\chi_j y^{(n-1)/2-ik}\psi_j^{(+)} - \omega_+^{(c)}(k)\sum_{j=1}^{N}\chi_j y^{(n-1)/2+ik}\widehat{\psi}_{j0}^{(+)}, \end{aligned}$$

where $\omega_\pm(k)$ and $\omega_\pm^{(c)}(k)$ are some functions of k.
(2) For any $\psi^{(-)}\in\mathbf{h}_\infty$, there exist a unique $\psi^{(+)}\in\mathbf{h}_\infty$ and $u\in\mathcal{N}(k)$, for which the expansion (1) holds. Moreover, $\widehat{S}(k):\mathbf{h}_\infty\ni\psi^{(-)}\to\psi^{(+)}\in\mathbf{h}_\infty$ is unitary.

The operator $\widehat{S}(k)$ is called the physical S-matrix, which is used in the study of inverse scattering from regular ends (cf. [**30**], [**13**]).

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4. Inverse scattering from cusp

4.1. Generalized S-matrix. We introduce the sequential spaces $\ell^{2,\pm\infty}$ by

$$\ell^{2,\infty} \ni a = (a_m)_{m\in\mathbf{Z}_+} \Longleftrightarrow \sum_{m\in\mathbf{Z}_+} |a_m|^2\rho^m < \infty, \quad \forall \rho > 1,$$

$$\ell^{2,-\infty} \ni b = (b_m)_{m\in\mathbf{Z}_+} \Longleftrightarrow \sum_{m\in\mathbf{Z}_+} |b_m|^2\rho^{-m} < \infty, \quad \exists \rho > 1,$$

Let $0 \neq k \in \mathbf{R}$. Suppose $u(x,y) \in C^\infty(M_j \times (1,\infty))$ and satisfies the the equation

$$-y^2\big(\partial_y^2 + \Delta_j\big)u - \frac{(n-1)^2}{4}u = k^2 y, \quad y > 1, \tag{17}$$

where Δ_j is the Laplacian on M_j with respect to the limiting metric $h_j^{(\infty)}$ or $h_j^{(0)}$ obtained when $y \to \infty$ or $y \to 0$ (cf. (3) or (4)).

Expanding u into a Fourier series

$$u(x,y) = \sum_{m\in\mathbf{Z}_+} u_m(y)\varphi_{j,m}(x),$$

we have

$$y^2\big(-\partial_y^2 + \lambda_{j,m}\big)u_m - \frac{(n-1)^2}{4}u_m = k^2 u_m, \quad y > 1.$$

Then u_m can be written as

$$u_m(y) = \begin{cases} a_m\, y^{(n-1)/2} I_{-ik}(\sqrt{\lambda_{j,m}}y) + b_m\, y^{(n-1)/2} K_{ik}(\sqrt{\lambda_{j,m}}y), & (m \neq 0), \\ a_0\, y^{(n-1)/2-ik} + b_0\, y^{(n-1)/2+ik}, & (m = 0). \end{cases} \tag{18}$$

Here $K_\nu(z)$, $I_\nu(z)$ are modified Bessel functions. Note the following exponential behaviors:

$$I_\nu(z) \sim \frac{1}{\sqrt{2\pi z}}e^z, \quad K_\nu(z) \sim \sqrt{\frac{\pi}{2z}}e^{-z}, \quad \text{as} \quad z \to \infty.$$

LEMMA 4.1. *Let $a = (a_m)_{m\in\mathbf{Z}_+}$, $b = (b_m)_{m\in\mathbf{Z}_+}$ be defined by (18). If $a \in l^{2,\infty}$, then $b \in l^{2,-\infty}$.*

We introduce the *spaces of generalized scattering data at infinity*:

$$\mathbf{A}_{\pm\infty} = \left(\bigoplus_{j=1}^{N} \ell^{2,\pm\infty}\right) \oplus \left(\bigoplus_{j=N+1}^{N+N'} L^2(M_j)\right). \tag{19}$$

We use the following notation. For

$$\psi^{(-)} = (a_1, \cdots, a_N, \psi_{N+1}^{(-)}, \cdots, \psi_{N+N'}^{(-)}) \in \mathbf{A}_\infty, \tag{20}$$

$$\psi^{(+)} = (b_1, \cdots, b_N, \psi_{N+1}^{(+)}, \cdots, \psi_{N+N'}^{(+)}) \in \mathbf{A}_{-\infty}, \tag{21}$$

let

$$u_j^{(-)} = \begin{cases} \omega_-^{(c)}(k)\Big(a_{j,0}\, y^{(n-1)/2-ik} \\ \qquad + \displaystyle\sum_{m=1}^{\infty} a_{j,m}\,\varphi_{j,m}(x) y^{(n-1)/2} I_{-ik}(\sqrt{\lambda_{j,m}}y)\Big), & 1 \le j \le N, \\ \omega_-(k)\, y^{(n-1)/2+ik}\psi_j^{(-)}(x), & N+1 \le j \le N+N', \end{cases} \tag{22}$$

$$u_j^{(+)} = \begin{cases} \omega_+^{(c)}(k)\Big(b_{j,0}\, y^{(n-1)/2+ik} \\ \qquad + \sum_{m=1}^{\infty} b_{j,m}\, \varphi_{j,m}(x) y^{(n-1)/2} K_{ik}(\sqrt{\lambda_{j,m}}y)\Big), \quad 1 \le j \le N, \\ \omega_+(k)\, y^{(n-1)/2-ik}\psi_j^{(+)}(x), \quad N+1 \le j \le N+N', \end{cases} \tag{23}$$

where $a_{j,m}, b_{j,m}$ are the m-th components of $a_j \in \ell^{2,\infty}, b_j \in \ell^{2,-\infty}$.

LEMMA 4.2. *Take $k > 0$ such that $k^2 \notin \sigma_p(H)$, and let $\psi^{(-)}$, $u_j^{(-)}$ be as in (20), (22). Then there exists a unique solution u such that*

$$(H - k^2)u = 0, \quad u - \sum_{j=1}^{N+N'} \widehat{\chi}_j u_j^{(-)} \in \mathcal{B}^*,$$

where $\widehat{\chi}_j(y) = 1$ for $y > 3$ and 0 for $y < 2$ when $1 \le j \le N$, and $\widehat{\chi}_j(y) = 1$ for $y < 1/3$ and 0 for $y > 1/2$ when $N+1 \le j \le N+N'$. Moreover, for this u, there exist $\psi^{(+)} \in \mathbf{A}_\infty$ and $u_j^{(+)}$ of the form (23) such that
(1) For $j = 1, \cdots, N$,

$$u = u_j^{(-)} - u_j^{(+)}, \quad \text{in} \quad M_j \times (3, \infty), \tag{24}$$

(2) For $j = N+1, \cdots, N+N'$,

$$u - u_j^{(-)} \simeq -u_j^{(+)}, \quad \text{in} \quad \mathcal{M}_j. \tag{25}$$

Explicitly, b_j's are given by

$$b_{j,0} = \mathcal{F}_j^{(+)}(k)f, \tag{26}$$

$$f = (H - k^2)u^{(-)}, \quad u^{(-)} = \sum_{j=1}^{N+N'} \widehat{\chi}_j u_j^{(-)}. \tag{27}$$

$$b_{j,m} = \int_2^\infty y^{(n-1)/2} I_{-ik}(\sqrt{\lambda_{j,m}}y) f_{j,m}(y) \frac{dy}{y^n}, \quad m \ge 1. \tag{28}$$

$$f_{j,m} = \langle f_j, \varphi_{j,m}\rangle_{L^2(M_j)}, \quad f_j = \chi_j f + [H_{free(j)}, \chi_j]R(k^2 + i0)f. \tag{29}$$

Here $H_{free(j)} = -y^2(\partial_y^2 + \Delta_j) - (n-1)^2/4$ is the unperturbed Laplacian for the end $\mathcal{M}_j$.

Given $u_j^{(-)}$, $j = 1, \cdots, N+N'$, one can obtain $b_{j,m}$ by observing the complete exponential asymptotic expansion of $u - u^{(j)}$ when $y \to \infty$. With this in mind, we make the following definition.

DEFINITION 4.3. *We call the operator*

$$\mathcal{S}(k) : \mathbf{A}_{-\infty} \ni \psi^{(-)} \to \psi^{(+)} \in \mathbf{A}_\infty$$

the generalized S-matrix.

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4.2. Splitting the manifold. We split $\mathcal{M}$ as

$$\mathcal{M} = \mathcal{M}_{ext} \cup \mathcal{M}_{int}, \quad \mathcal{M}_{ext} = M_1 \times (2,\infty), \quad \mathcal{M}_{int} = \mathcal{M} \setminus (M_1 \times [2,\infty)), \tag{30}$$

Thus, $\mathcal{M}_{ext}$ and $\mathcal{M}_{int}$ have common boundary $\Gamma = M_1 \times \{2\}$. Recall that the end $\mathcal{M}_1$ has a cusp, and $\mathcal{M}_{ext}$ is a direct product of M_1 and $(2,\infty)$.

Let Δ_g be the Laplace-Beltrami operator on $\mathcal{M}$, H_{ext} and H_{int}, respectively, be $-\Delta_g - (n-1)^2/4$ defined on $\mathcal{M}_{ext}$, $\mathcal{M}_{int}$ with Neumann boundary condition on Γ. If $\mathcal{M}$ has only one end (i.e. $N + N' = 1$), $\mathcal{M}_{int}$ is a compact manifold, and H_{int} has a discrete spectrum. If $N \geq 2$, both of $\mathcal{M}_{int}$ and $\mathcal{M}_{ext}$ are non-compact, and the theorems in §4 also hold in this case. We denote the inner product of $L^2(\Gamma)$ by $\langle f, g\rangle_\Gamma = \displaystyle\int_\Gamma f\overline{g}\, d\Gamma$.

We put

$$\Phi_m^{(0)} = \begin{cases} y^{(n-1)/2-ik}|M_1|^{-1/2}, & m = 0, \\ y^{(n-1)/2} I_{-ik}(\sqrt{\lambda_{1,m}}y)\varphi_{1,m}(x), & m \neq 0, \end{cases}$$

$$g_m = (H - k^2)\chi_1 \Phi_m^{(0)} = [H_{free(1)}, \chi_1]\Phi_m^{(0)},$$

$$\Phi_m = \chi_1 \Phi_m^{(0)} - R(k^2 + i0) g_m. \tag{31}$$

LEMMA 4.4. *Let $k > 0$ and $k^2 \notin \sigma_p(H) \cap \sigma_p(H_{int})$. If $f \in L^2(\Gamma)$ satisfies*

$$\langle f, \partial_\nu \Phi_m\rangle_\Gamma = 0, \quad \forall m \in \mathbf{Z}_+, \tag{32}$$

where ν is the unit normal to Γ, then $f = 0$.

The generalized S-matrix $\mathcal{S}(k)$ is an operator-valued $(N + N') \times (N + N')$ matrix. Let $\mathcal{S}_{11}(k)$ be its $(1,1)$ entry. For $a \in \ell^{2,\infty}$, we put $b = \mathcal{S}_{11}(k)a \in \ell^{2,-\infty}$, and

$$\Phi = \sum_{m \in \mathbf{Z}_+} a_m \Phi_m.$$

Then $(H - k^2)\Phi = 0$ and in $\mathcal{M}_1$,

$$\Phi = u_1^{(-)} - u_1^{(+)},$$

$$u_1^{(-)} = \omega_-^{(c)}(k)\Big(a_0 y^{(n-1)/2-ik} + \sum_{m \geq 1} a_m \varphi_{1,m}(x) y^{(n-1)/2} I_{-ik}(\sqrt{\lambda_{1,m}}y)\Big),$$

$$u_1^{(+)} = \omega_+^{(c)}(k)\Big(b_0 y^{(n-1)/2+ik} + \sum_{m \geq 1} b_m \varphi_{1,m}(x) y^{(n-1)/2} K_{ik}(\sqrt{\lambda_{1,m}}y)\Big).$$

Therefore, determination of $\mathcal{S}_{11}(k)$ is equivalent to the observation of the outgoing exponentially decaying wave $u_1^{(+)}$ at $\mathcal{M}_1$ for any incoming exponentially growing wave $u_1^{(-)}$ sent into the cusp $\mathcal{M}_1$.

4.3. Gel'fand problem, BSP and N-D map. Let (Ω, g) be a compact Riemannian manifold with boundary $\Gamma = \partial\Omega$, and $-\Delta_g$ the associated Laplace-Beltrami operator. Let $0 = \lambda_1 < \lambda_2 < \cdots$ be its Neumann eigenvalues without counting multiplicities, and $\varphi_{i,1}, \cdots, \varphi_{i,m(i)}$ be the orthonormal system of eigenvectors associated with the eigenvalue λ_i. Let us call the set

$$\Big\{(\lambda_i, \varphi_{i,1}\big|_\Gamma, \cdots, \varphi_{i,m(i)}\big|_\Gamma)\Big\}_{i=1}^\infty$$

the boundary spectral data (**BSD**). The problem raised by Gel'fand is:

Does BSD determine Ω and the Riemannian metric g on Ω?

This problem was solved by Belishev-Kurylev [**4**] using the boundary control method (BC-method) proposed by Belishev [**3**]. For the recent developments of this reconstruction method, see [**2**, **16**, **18**, **19**], and for the related methods at a fixed frequency inverse problems, see [**21**, **22**, **24**]. Although it is formulated in terms of BSD, what is actually used in the BC-method is the boundary spectral projection (**BSP**) defined by $\left(\Gamma, \left\{(\lambda_i, \sum_{j=1}^{m(i)} \varphi_{i,j}(x)\overline{\varphi_{i,j}(y)}\big|_{(x,y)\in\Gamma\times\Gamma}\right\}_{i=1}^{\infty}\right)$. This appears in the integral kernels the *Neumann to Dirichlet map (N-D map)* $\Lambda(z) : f \to u\big|_\Gamma$, where u is the solution to the Neumann problem

$$\begin{cases} (-\Delta_g - z)u = 0 \quad \text{in} \quad \Omega, \\ \partial_\nu u = f \in H^{-1/2}(\Gamma), \end{cases} \tag{33}$$

ν being the outer unit normal to Γ, $z \notin \sigma(-\Delta_g)$. Indeed, $z \mapsto \Lambda(z)$ is an operator-valued meromorphic function that has poles at the eigenvalues λ_j and the residues of the function $\Lambda(z)$ are finite dimensional operators which integral kernels are given by the BSP, see [**17**]. The N-D map is related to the resolvent $(-\Delta_g - z)^{-1}$ in the following way:

$$\Lambda(z) = \delta_\Gamma^*(-\Delta_g - z)^{-1}\delta_\Gamma, \quad z \notin \sigma(-\Delta_g). \tag{34}$$

Here $\delta_\Gamma \in \mathbf{B}(H^{-1/2}(\Gamma); H^{-1}(\Omega))$ is the adjoint of the trace operator

$$r_\Gamma : H^1(\Omega) \ni w \to w\big|_\Gamma \in H^{1/2}(\Gamma),$$

$$(\delta_\Gamma f, w)_{L^2(\Omega)} = (f, r_\Gamma w)_{L^2(\Gamma)}, \quad f \in H^{-1/2}(\Gamma), \quad w \in H^1(\Omega). \tag{35}$$

LEMMA 4.5. *If $\Omega = \mathcal{M}_{int}$ of form (30), the knowledge of BSP is equivalent to the knowledge of the N-D map $\Lambda(z)$ for all $z \notin \sigma(-\Delta_g)$.*

4.4. Generalized S-matrix and N-D map. Let $\Lambda(z)$ be the N-D map for $\Omega = \Omega_{int}$. Now suppose we are given two orbifolds $\mathcal{M}^{(i)}$, $i = 1, 2$, satisfying the assumptions (A-1) $\sim$ (A-3) in §1. Let $H^{(i)}$ be the shifted Laplacian in $\mathcal{M}^{(i)}$. Assume that $\mathcal{M}^{(i)}$ has $N_i + N_i'$ ends, $N_i > 0$, and let $\mathcal{S}_{11}^{(i)}(k)$ be the $(1,1)$ component of the generalized S-matrix for $H^{(i)}$. Let $(\mathcal{M}_1^{(i)}, h_1^i), i = 1, 2$, be isometric Riemannian orbifolds. Thus, we can naturally identify $\mathcal{M}_1^{(i)}, i = 1, 2$. Next we split $\mathcal{M}^{(i)}$ into $\mathcal{M}_{int}^{(i)} \cup \mathcal{M}_{ext}^{(i)}$ as above using $\Gamma^{(1)} = \Gamma^{(2)}$. Let $H_{int}^{(i)}$ be the Laplace-Beltrami operator of $\mathcal{M}_{int}^{(i)}$ with the Neumann boundary condition on $\Gamma^{(i)}$, and define the N-D map $\Lambda^{(i)}(z)$ for $\mathcal{M}_{int}^{(i)}$. With this preparation, we can prove the following lemma.

LEMMA 4.6. *If $\mathcal{S}_{11}^{(1)}(k) = \mathcal{S}_{11}^{(2)}(k)$ for $k > 0$, $k^2 \notin \sigma_p(H^{(1)}) \cup \sigma_p(H^{(2)})$, we have*

$$\Lambda^{(1)}(k^2) = \Lambda^{(2)}(k^2), \quad \forall k^2 \in (0,\infty) \setminus \sigma_p(H_{int}^{(1)}) \cup \sigma_p(H_{int}^{(2)}).$$

In particular, BSP's for $H_{int}^{(1)}$ and $H_{int}^{(2)}$ coincide.

5. Orbifold isomorphism

Above we have reduced the inverse scattering problem for the construction of an orbifold from local measurements. This problem is studied in detail in [**20**] in the general n-dimensional case and in the 2-dimensional case, in the context of scattering problems, in [**14**]. We give an outline of the proof of Theorem 1.1 that is based on the basic steps of §5 in [**14**], and with modifications necessary to deal with the multidimensional, rather than 2D, case.

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Observe that $\Lambda(z)$ is an integral operator with the kernel $G_{int}(X,Y;z)$, where $X=(x,2), Y=(x',2)$, $x,x'\in\Gamma$, where $G_{int}(\cdot,\cdot;z)$ is Green's function for the Neumann problem in $\mathcal{M}_{int}$. The function $G_{int}(X,Y;z)$, $X,Y\in\mathcal{M}_{int}$, enjoys the following separation property: If $G_{int}(X,Y;z)=G_{int}(X',Y;z)$ for all $Y\in\Gamma$, $z\in\mathbf{C}\setminus\mathbf{R}$, then $X=X'$.

The proof of Theorem 1.1 consists of two principal steps:

First, we show that $\mathcal{M}_{int}^{(i),reg}$ are isometric and, since $\mathcal{M}_{int}^{(i)}$ is the closure of $\mathcal{M}_{int}^{(i),reg}$, $i=1,2$, $\mathcal{M}_{int}^{(i)}$ are isometric as metric spaces. In the future, we refer to this isometry as $\mathbf{X}:\mathcal{M}_{int}^{(1)}\to\mathcal{M}_{int}^{(2)}$ and, in the first step, we recover $\mathbf{X}$ in an inductive procedure.

Next, we use the fact that, if two oriented orbifolds are isometric as metric spaces, then they are orbifold isometric. This means that $p^{(1)}\in\mathcal{M}_{int}^{(1),sing}$ if and only if $p^{(2)}=\mathbf{X}(p^{(1)})\in\mathcal{M}_{int}^{(2),sing}$, and the groups $G_{p^{(1)}}$ and $G_{p^{(2)}}$ are isomorphic.

The proof of the first step is made by inductively enlarging the parts of $\mathcal{M}_{int}^{(i),reg}$ which are isometric to each other by starting from $\Gamma=\Gamma^{(1)}=\Gamma^{(2)}$. Actually, we already know from (3) and the assumption of the theorem, $M_1^{(1),reg}\times(1,2)$ and $M_1^{(2),reg}\times(1,2)$ are isometric. Let us call the parts of $\mathcal{M}_{int}^{(i),reg}$ which are already proven to be isometric after m iterations by $\Omega_m^{(i)}$. It would always be the case that $\Omega_m^{(i)}\subset\mathcal{M}_{int}^{(i),reg}$ are arcwise connected with Γ. Then, from Lemma 4.6, we see that

$$G_{int}^{(2)}(\mathbf{X}(X),\mathbf{X}(Y);z)=G_{int}^{(1)}(X,Y;z),\quad X,Y\in\Omega_m^{(1)},\quad z\in\mathbf{C}\setminus\mathbf{R}. \tag{36}$$

The induction step is based on the possibility to extend the isometry $\mathbf{X}:\Omega_m^{(1)}\to\Omega_m^{(2)}$ onto a larger set $\mathbf{X}:\Omega_{m+1}^{(1)}\to\Omega_{m+1}^{(2)}$. To explain this procedure, let $B_\delta(p^{(i)})$ be the ball of radius δ in $\Omega_m^{(i)}$ with $B_\delta(p^{(2)})=\mathbf{X}(B_\delta(p^{(1)}))$. Then, using the variant of the BC-method explained in e.g. [**14**], we show $G^{(i)}(X^{(i)},Y^{(i)};z)$, $X^{(i)},Y^{(i)}\in B_\delta(p^{(i)})$, determines $r_i=\mathrm{inj}(p^{(i)})$ and the Riemannian structure, in normal coordinates, of $B_{r_i}(p^{(i)})$. Since (36) is satisfied for $X^{(i)},Y^{(i)}\in B_\delta(p^{(i)})$, we see that $r_1=r_2=r$, and there is an isomorphism $\mathbf{X}$ from $B_r(p^{(1)})$ to $B_r(p^{(2)})$. Take $\Omega_{m+1}^{(i)}=\Omega_m^{(i)}\cup B_r(p^{(i)})$. Then $G^{(i)}(X^{(i)},Y^{(i)};z)$ is uniquely extended to $X^{(i)},Y^{(i)}\in\Omega_{m+1}^{(i)}$. Using the separtion property, this means that $\mathbf{X}$ can be extended as an isomorphism from $\Omega_{m+1}^{(1)}$ to $\Omega_{m+1}^{(2)}$. Note that if $p^{(i)}\in\mathcal{M}_{int}^{(i),reg}$, then $\mathrm{inj}(p^{(i)})\le d(p^{(i)},\mathcal{M}_{int}^{(i),sing})$ so that $\Omega_{m+1}^{(i)}\subset\mathcal{M}_{int}^{(i),reg}$. Standard Kuratowski-Zorn arguments show that $\mathbf{X}$ can be extended to an isometry from $\mathcal{M}_{int}^{(1),reg}$ to $\mathcal{M}_{int}^{(2),reg}$.

The second step, regarding the orbifold isomorphism of $\mathcal{M}_{int}^{(i)}$ can be carried out following the same considerations as in the proof of Theorem 9.1 in [**20**]. Note that, although Theorem 9.1 is proven only for the compact orbifolds without boundary, it can be easily extended to the considered case, since the structure of $\mathcal{M}_{int}^{(i)}\cap\big(M_1^{(i)}\times(1,2)\big)$ is known, see (3), and the constructions in [**20**] is local. □

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Error estimates of the Bloch band-based Gaussian beam superposition for the Schrödinger equation

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Dedicated to our friend James Ralston

Abstract. This work is concerned with asymptotic approximations of the semi-classical Schrödinger equation in periodic media using Gaussian beams. For the underlying equation, subject to a highly oscillatory initial data, a hybrid of the Gaussian beam approximation and homogenization leads to the Bloch eigenvalue problem and associated evolution equations for Gaussian beam components in each Bloch band. We formulate a superposition of Bloch-band based Gaussian beams to generate high frequency approximate solutions to the original wave field. For initial data of a sum of finite number of band eigen-functions, we prove that the first-order Gaussian beam superposition converges to the original wave field at a rate of $\epsilon^{1/2}$, with ϵ the semiclassically scaled constant, as long as the initial data for Gaussian beam components in each band are prepared with same order of error or smaller. For a natural choice of initial approximation, a rate of $\epsilon^{1/2}$ of initial error is verified.

1. Introduction

We consider the semiclassically scaled Schrödinger equation with a periodic potential:

$$i\varepsilon\partial_t\Psi = -\frac{\varepsilon^2}{2}\Delta\Psi + V\left(\frac{x}{\varepsilon}\right)\Psi + V_e(x)\Psi, \quad x\in\mathbb{R}^d, \quad t>0, \tag{1.1}$$

subject to the two-scale initial condition:

$$\Psi(0,x) = g\left(x,\frac{x}{\varepsilon}\right)e^{iS_0(x)/\varepsilon}, \quad x\in\mathbb{R}^d, \tag{1.2}$$

where $\Psi(t,x)$ is a complex wave function, ε is the re-scaled Planck constant, $V_e(x)$– given external potential, $S_0(x)$– real-valued function, $g(x,y) = g(x,y+2\pi)$ – a periodic function in y, compactly supported in x, i.e., $g(x,y)=0,\ x\notin K_0,\ K_0$– is a bounded set. $V(y)$ is periodic with respect to the crystal lattice $\Gamma = (2\pi\mathbb{Z})^d$, it models the electronic potential generated by the lattice of atoms in the crystal [**14**].

A typical application arises in solid state physics where (1.1) describes the quantum dynamics of Bloch electrons moving in a crystalline lattice (generated by the ionic cores) [**40**]. The asymptotics of (1.1) as $\varepsilon\to 0+$ is a well-studied two-scale problem in the physics and mathematics literature [**1**, **8**, **13**, **14**, **16**, **22**, **23**, **35**, **42**].

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On the other hand, the computational challenge because of the small parameter ε has prompted a search for asymptotic model based numerical methods, see e.g., [**25**, **32**].

The main feature of this type of problems is the "band structure" of solutions. For suitable initial data, the solution depends on the semi-classical Hamiltonian operator

$$H(k,y) = \frac{1}{2}(-i\nabla_y + k)^2 + V(y), \quad y \in \Gamma, \tag{1.3}$$

and the solution of the eigenvalue problem:

$$\begin{cases} H(k,y)z(k,y) = E(k)z(k,y), \\ z(k,y) = z(k,y+2\pi), \end{cases} \tag{1.4}$$

where $k \in [-1/2, 1/2]^d$– called Brillouin zone, see [**47**]. The behavior of the eigenpairs for general k can be characterized by that for k in this zone through a periodic extension.

According to the theory of Bloch waves [**46**], the self-adjoint semi-bounded operator $H(k,y)$ with a compact resolvent has a complete set of orthonormal eigenfunctions $z_n(k,y)$ in L^2, with $e^{iky}z_n(k,y)$ called Bloch functions. The correspondent eigenvalues $E_n(k)$ are called band functions. Standard perturbation theory [**26**] shows that $E_n(k)$ is a continuous function of k and real analytic in a neighborhood of any k such that

$$E_{n-1}(k) < E_n(k) < E_{n+1}(k). \tag{1.5}$$

The proof has been given first in [**21**] and [**9**, **10**] for $d = 1$ and in [**34**] for $d = 3$. We assume that (1.5) is satisfied, i.e., all band functions are strictly separated, $\forall n,\ k$. Under this assumption one can choose $z_n(k,y)$ associated to $E_n(k)$ to be real analytic functions of k [**14**]. This allows for a unique analytic extension of both $z_n(k,y)$ and $E_n(k)$ so that they can be evaluated for some complex k, say $k = \partial_x\Phi$, where Φ is the Gaussian beam phase.

A classical approach to solve this problem asymptotically is by the Bloch band decomposition based WKB method [**6**, **18**, **41**], which leads to Hamilton-Jacobi and transport equations valid up to caustics. The Bloch-band based level set method was introduced in [**32**] to compute crossing rays and position density beyond caustics. However, at caustics, neither method gives correct prediction for the amplitude. A closely related alternative to the WKB method is the construction of approximations based on Gaussian beams. Gaussian beams are asymptotic solutions concentrated on classical trajectories for the Hamiltonian, and they remain valid beyond "caustics". The existence of Gaussian beam solutions has been known since sometime in the 1960's, first in connection with lasers, see Babič and Buldyrev [**2**, **3**]. Later, they were used to obtain results on the propagation of singularities in solutions of PDEs [**21**, **37**]. The idea of using sums of Gaussian beams to represent more general high frequency solutions was first introduced by Babič and Pankratova in [**4**] and was later proposed as a method for wave propagation by Popov in [**36**]. At present there is considerable interest in using superpositions of beams to resolve high frequency waves near caustics. This goes back to the geophysical applications in [**12**, **20**]. Recent work in this direction includes [**24**, **25**, **28**, **33**, **38**, **43**, **44**].

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The accuracy of the Gaussian beam superposition to approximate the original wave field is important, but determining the error of the Gaussian beam superposition is highly non-trivial, see the conclusion section of the review article by Babič and Popov [**5**]. In the past few years, some significant progress on estimates of the error has been made. One of the first results was obtained by Tanushev for the initial error in 2008 [**43**]. Liu and Ralston [**29**, **30**] gave rigorous convergence rates in terms of the small wave length for both the acoustic wave equation in the scaled energy norm and the Schrödinger equation in the L^2 norm. At about the same time, error estimates for phase space beam superposition were obtained by Bougacha, Akian and Alexandre in [**7**] for the acoustic wave equation. Building upon these advances, Liu, Runborg and Tanushev further obtained optimal estimates for a class of high-order, strictly hyperbolic partial differential equations [**31**].

Other methods that also yield an asymptotic description for time-scales of order $O(1)$ (i.e. beyond caustics) have been developed such as those based on Wigner measures [**15**]. The dynamics of the Wigner function corresponding to the Schrödinger wave function can be semiclassically approximated to an error of order $O(\epsilon)$, see [**45**] and references to previous works therein. More recently, so-called space-adiabatic perturbation theory has been used to derive an effective Hamiltonian, governing the dynamics of particles in periodic potentials under the additional influence of slowly varying perturbations [**23**, **35**]. The semi-classical asymptotics of this effective model is then obtained in a second step, invoking an Egorov-type theorem. Another analogous approach is the propagation of the so called semiclassical wave packets, developed by Hagedorn et al. [**19**]. A recent rigorous analysis is given by Carles and Sparber [**11**] in the context of the Schrödinger equation with periodic potentials. There the authors prove that using semiclassical wave packets within each Bloch band, an approximation result up to errors of order $O(\epsilon^{1/2})$ can be achieved, but for times up to the Ehrenfest time-scale $T\ \ln(\frac{1}{\varepsilon})$.

In this paper, we develop a convergence theory for the Gaussian beam superposition as a valid approximate solution of problem (1.1)–(1.2). The novel contribution of the present work lies in the accuracy justification for an explicit construction—the Gaussian beam superposition. Indeed, Gaussian beam methods are widely used in numerical simulations of high frequency waves fields.

The Gaussian beam construction is based on Gaussian beams in each Bloch band, and carried out by using the two scale expansion approach, essentially following DiMassi et al. [**14**] for adiabatic perturbations. The accuracy study in [**14**] was only on how well each Gaussian beam asymptotically satisfies the PDE. In order to handle more general initial data in this paper, we (i) present the approximation solution through beam superpositions over Bloch bands and initial points from which beams are issued; and (ii) estimate the error between the exact wave field and the asymptotic ones. Numerical results using this type of superpositions were presented in [**25**].

Our focus in this work is mainly on (ii). We use the notation: $f \in C_b^m(\mathbb{R}^d)$ means that f is m times differentiable function, and all derivatives up to m-th order included are bounded functions in $\mathbb{R}^d$. $f \in L_x^2$ means that f belongs to $L^2(\mathbb{R}^d)$ in x variable. The main result can be stated as follows.

THEOREM 1.1. *Suppose that $S_0 \in C_b^3(\mathbb{R}^d), V_e \in C_b^{d+4}(\mathbb{R}^d)$, both $V(y)$ and $g(x,y)$ are periodic in y with respect to the crystal lattice $\Gamma = (2\pi\mathbb{Z})^d$, also $V \in C^2(\mathbb{R}^d)$ and $g(x,y)$ has compact support in x. We also assume that g has the*

following expression

$$g(x,y)=\sum_{n=1}^{N}a_n(x)z_n(\nabla_x S_0(x),y),$$

where $z_n(k,y)$ *are eigen-functions of* (1.4) *with eigenvalues* $E_n(k)$ *satisfying* (1.5). *Let* $\Psi(t,x)$ *be the solution to* (1.1)-(1.2), *and*

$$\Psi^{\epsilon}(t,x)=\tilde{\Psi}^{\varepsilon}\left(t,x,\frac{x}{\varepsilon}\right)$$

be the Gaussian beam superposition defined by (3.37) *for* $0<t\le T$, *then*

$$\|\Psi-\Psi^{\epsilon}\|_{L^2_x}\le C\varepsilon^{1/2},$$

where C *may depend on* T, N *and data given, but independent of* ε.

REMARK 1.1. *The regularity requirement of* V *is sufficient for validating the Gaussian beam approximation, but excludes the Coulomb-like singularity which is typical of the mean field electrostatic potential in real solids. It would be interesting to investigate how such an assumption could be relaxed.*

We prove this result in several steps. We first reformulate the problem using the two scale expansion method [**6**, **14**], in which both x and $y=\frac{x}{\varepsilon}$ are regarded as two independent variables. The well-posedness estimate for this reformulated problem tells that the total error is bounded by the sum of initial and evolution error. For initial error, we use some techniques similar to those developed by Tanushev [**43**], except that here we have to deal with the band structure. The band structure induces additional technical difficulties, which we solve in several steps. As for evolution error part, we rely on the non-squeezing argument proved in [**31**], which is the key technique for the proof. After we obtain estimate in $L^2_{x,y}$ we convert to L^2_x.

This paper has the following structure: in section 2 we use the two scale method to reformulate our problem and state the corresponding results; in the end of this section we prove Theorem 1.1 for the original problem. In section 3 we review Gaussian beam constructions and formulate our Gaussian beam superposition. Justifications of main results are presented in section 4 and section 5. In section 6 we discuss possible extensions of our results and some remaining challenges.

2. Set-up and main results

In order to construct an asymptotic solution of (1.1) we use the two-scale method as in [**6**, **14**]. We regard x and $y=\dfrac{x}{\varepsilon}$ as independent variables and introduce a new function

$$\tilde{\Psi}(t,x,y)\equiv\Psi(t,x),$$

equation (1.1) can be rewritten in the form:

$$\begin{cases} i\varepsilon\partial_t\tilde{\Psi}=-\frac{1}{2}(\varepsilon\nabla_x+\nabla_y)^2\tilde{\Psi}+V(y)\tilde{\Psi}+V_e(x)\tilde{\Psi},\\ \tilde{\Psi}(0,x,y)=g(x,y)e^{iS_0(x)/\varepsilon}, \quad x\in\mathbb{R}^d, \quad y\in[0,2\pi]^d. \end{cases} \tag{2.1}$$

We assume that the initial amplitude $g(x,y)$ can be decomposed into N bands,

$$g(x,y)=\sum_{n=1}^{N}a_n(x)z_n(\nabla_x S_0,y), \tag{2.2}$$

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where a_n is determined by

$$a_n(x) = \int_{[0,2\pi]^d} g(x,y)\overline{z_n(\nabla_x S_0, y)}dy, \tag{2.3}$$

and $\left\{z_n(\partial_x S_0, y)\right\}_{n=1}^{\infty}$ are eigenfunctions of the self-adjoint second order differential operator $H(k,y)$ defined by (1.3). $\left\{z_n(\partial_x S_0, y)\right\}_{n=1}^{\infty}$ form an orthonormal basis in $L^2(0,2\pi)$.

For each energy band, the Gaussian beam ansatz was constructed in [**14**], which we will review in section 3:

$$\tilde{\Psi}^n_{GB}(t,x,y;x_0) = A^n(t,x,y;x_0)e^{i\Phi_n(t,x;x_0)/\varepsilon}, \tag{2.4}$$

where Φ_n and A^n are Gaussian beam phases and amplitudes, respectively, $n = 1,\dots N$. The Gaussian beam phase is defined as:

$$\begin{aligned}\Phi_n(t,x;x_0) &= S_n(t;x_0) + p_n(t;x_0)(x-\tilde{x}_n(t;x_0)) \\ &\quad + \frac{1}{2}(x-\tilde{x}_n(t;x_0))^\top M_n(t;x_0)(x-\tilde{x}_n(t;x_0)),\end{aligned} \tag{2.5}$$

where $\tilde{x}_n, p_n, S_n$ and M_n, as well as the amplitude a_n satisfy corresponding evolution equations (see section 3 for details). Using the fact that the Schrödinger equation is linear, we sum the Gaussian beam ansatz for each band to obtain the approximate solution along the ray:

$$\tilde{\Psi}_{GB}(t,x,y;x_0) = \sum_{n=1}^{N} \tilde{\Psi}^n_{GB}(t,x,y;x_0). \tag{2.6}$$

Using $\tilde{\Psi}_{GB}(t,x,y;x_0)$ as a building block of the approximate solution, we have the following superposition of Gaussian beams:

$$\tilde{\Psi}^\varepsilon(t,x,y) = \frac{1}{(2\pi\varepsilon)^{\frac{d}{2}}}\int_{K_0} \tilde{\Psi}_{GB}(t,x,y;x_0)dx_0, \tag{2.7}$$

where $\dfrac{1}{(2\pi\varepsilon)^{\frac{d}{2}}}$ is a normalizing constant which is needed for matching the initial data of problem (2.1). The initial data is approximated by:

$$\tilde{\Psi}^\varepsilon(0,x,y) = \frac{1}{(2\pi\varepsilon)^{\frac{d}{2}}}\int_{K_0} \sum_{n=1}^{N} A^n(0,x,y;x_0)e^{i\Phi^0(x;x_0)/\varepsilon}dx_0, \tag{2.8}$$

where $A^n(0,x,y;x_0)$ is the initial data for the amplitude, and Φ^0 is the initial Gaussian beam phase for all bands, chosen as follows:

$$\Phi^0(x;x_0) = S_0(x_0) + \nabla_x S_0(x_0)\cdot(x-x_0) + \frac{1}{2}(x-x_0)^\top\cdot(\nabla_x^2 S_0(x_0) + iI)(x-x_0). \tag{2.9}$$

We address the two-scale problem, with $y = \dfrac{x}{\varepsilon}$ considered to be independent variables, and then convert to the original problem. The norm $L^2_{x,y}$ is defined as follows:

$$\|u\|^2_{L^2_{x,y}} = \int_{[0,2\pi]^d}\int_{\mathbb{R}^d} |u(x,y)|^2 dxdy. \tag{2.10}$$

We obtain two major results formulated in the following theorems:

THEOREM 2.1. *[Initial error estimate] Let $K_0 \subset \mathbb{R}^d$ be a bounded measurable set, $g(x,y) \in H^1(K_0 \times [0,2\pi]^d)$, $S_0(x) \in C_b^3(\mathbb{R}^d)$. Then the initial error made by the Gaussian beam superposition (2.8) is as follows:*

$$\|\tilde{\Psi}(0,x,y) - \tilde{\Psi}^\varepsilon(0,x,y)\|_{L^2_{x,y}} \le C\varepsilon^{1/2},$$

where constant C depends only on the initial amplitude $g(x,y)$ and the initial phase $S_0(x)$.

The proof is split in two parts, see Lemma 4.1 and Lemma 4.2.

In order to measure the evolution error, we define P the two-scale Schrödinger operator,

$$P(\tilde{\Psi}) = i\varepsilon\partial_t\tilde{\Psi} + \frac{1}{2}(\varepsilon\nabla_x + \nabla_y)^2\tilde{\Psi} - V(y)\tilde{\Psi} - V_e(x)\tilde{\Psi}. \tag{2.11}$$

THEOREM 2.2. *[Evolution error estimate] Let K_0 be a bounded set, condition (1.5) is satisfied, the external potential $V_e(x) \in C_b^{d+4}(\mathbb{R}^d)$. Then the evolution error is*

$$\sup_{0\le t\le T}\|P(\tilde{\Psi}^\varepsilon(t,\cdot))\|_{L^2_{x,y}} \le C\varepsilon^{3/2},$$

where constant C depends on the measure of set K_0, finite time T, the number of bands N, and external potential V_e.

The proof of this theorem is done in several steps, one step requires a phase estimate which uses essentially the "Non-squeezing" result obtained by Liu et al. [**31**].

Finally, we recall the well-posedness estimate for the two-scale Schrödinger equation (2.1) (see, e.g., [**39**, p. 134]).

LEMMA 2.1. *The L^2–norm of the difference between the exact solution $\tilde{\Psi}$ and an approximate solution $\tilde{\Psi}^\varepsilon$ of the problem (2.1) is bounded above by the following estimate:*

$$\begin{aligned}\|\tilde{\Psi}(t,x,y) - \tilde{\Psi}^\varepsilon(t,x,y)\|_{L^2_{x,y}} &\le \|\tilde{\Psi}(0,x,y) - \tilde{\Psi}^\varepsilon(0,x,y)\|_{L^2_{x,y}} \\ &\quad + \frac{1}{\varepsilon}\int_0^T \|P(\tilde{\Psi}^\varepsilon)\|_{L^2_{x,y}}dt, \quad 0 < t \le T,\end{aligned} \tag{2.12}$$

where T is a finite time, $\tilde{\Psi}(0,\cdot), \tilde{\Psi}^\varepsilon(0,\cdot)$ are initial values of the exact and approximate solution respectively.

This result when combined with both initial error and evolution error gives the following.

COROLLARY 2.1. *The total error made by the first order Gaussian beam superposition method is of order $\varepsilon^{1/2}$ in the following sense*

$$\|\tilde{\Psi} - \tilde{\Psi}^\varepsilon\|_{L^2_{x,y}} \le C\varepsilon^{1/2}.$$

In order to convert the two-scale result stated in Corollary 2.1 to the original problem, we prepare the following lemma.

LEMMA 2.2. *Assume that $f(x,y) \in L^2(\mathbb{R}^d, [-\pi,\pi]^d)$ and f is 2π periodic in y. Then for sufficiently small ε,*

$$\left\|f\left(x, \frac{x}{\varepsilon}\right)\right\|_{L^2_x} \le \frac{1}{\pi^{\frac{d}{2}}}\|f(x,y)\|_{L^2_{x,y}}. \tag{2.13}$$

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PROOF. Denote $Y_\varepsilon^k = [2\pi k\varepsilon, 2\pi(k+1)\varepsilon]^d$ and let $I_\varepsilon = \{k \in \mathbb{Z}^d, \quad Y_\varepsilon^k \cap [-R,R]^d \neq \emptyset\}$ for any fixed $R > 0$. Then,

$$\int_{|x|\leq R} f^2\left(x, \frac{x}{\varepsilon}\right) dx \leq \sum_{k\in I_\varepsilon} \int_{Y_\varepsilon^k} f^2\left(x, \frac{x}{\varepsilon}\right) dx.$$

Here $|x|$ denotes l^∞– norm of the vector x, hence $|x| \leq R$ corresponds to a d-dimensional cube. Introducing a change of variable $y = \frac{x}{\varepsilon}$ and taking advantage of the periodicity in y, one can rewrite the right hand side of the above expression in the shifted cell form:

$$\int_{|x|\leq R} f^2\left(x, \frac{x}{\varepsilon}\right) dx \leq \sum_{k\in I_\varepsilon} \varepsilon^d \int_{|y|\leq\pi} f^2(\varepsilon(y+2\pi k), y) dy.$$

For fixed y the right hand side corresponds to the Riemann sum of the function

$$g^2(x) = \int_{|y|\leq\pi} f^2(x+\varepsilon y, y) dy$$

sampled at $x_k = 2\pi k\varepsilon$. Note that the step size in all direction $\Delta x_k = (2\pi\varepsilon)^d$, hence

$$\begin{aligned}\sum_{k\in I_\varepsilon} \varepsilon^d \int_{|y|\leq\pi} f^2(\varepsilon(y+2\pi k), y) dy &= \frac{1}{(2\pi)^d} \sum_{k\in I_\varepsilon} g^2(x_k)\Delta x_k \\ &\to \frac{1}{(2\pi)^d} \int_{|x|\leq R} \int_{|y|\leq\pi} f^2(x,y) dy dx \quad \text{as} \quad \varepsilon \to 0,\end{aligned}$$

with the first order of convergence. Therefore,

$$\int_{|x|\leq R} f^2\left(x, \frac{x}{\varepsilon}\right) dx \leq \frac{1}{(2\pi)^d} \int_{|x|\leq R} \int_{|y|\leq\pi} f^2(x,y) dy dx + C\varepsilon.$$

Taking $\varepsilon = C^{-1}(2\pi)^{-d}\|f\|^2_{L^2_{x,y}}$, then the right hand side is bounded above by

$$\frac{1}{2^{d-1}\pi^d} \int_{\mathbb{R}} \int_{|y|\leq\pi} f^2(x,y) dy dx.$$

Passing limit $R \to \infty$ leads to the desired estimate (2.13). □

Set the error in two scale setting as

$$e(t,x,y) = \tilde{\Psi}(t,x,y) - \tilde{\Psi}^\varepsilon(t,x,y),$$

then the error in original variable gives

$$\Psi(t,x) - \Psi^\epsilon(t,x) = e(t,x,x/\varepsilon).$$

Applying Lemma 2.2 and using Corrolary 2.1 we prove Theorem 1.1 for the original problem.

3. Construction

In this section we first review the classical asymptotic approach and the band structure, then the Gaussian beam construction following [**14**]. For simplicity, the construction and proofs are presented in one-dimensional setting.

Asymptotic Approach. We look for an approximate solution to (2.1) of the form:

$$\tilde{\Psi}^\varepsilon(t,x,y) = A(t,x,y)e^{i\Phi(t,x)/\varepsilon}, \tag{3.1}$$

where

$$A(t,x,y) = A_0(t,x,y) + A_1(t,x,y)\varepsilon + \cdots + A_l(t,x,y)\varepsilon^l,$$

with A_i satisfying:

$$A_i(t,x,y) = A_i(t,x,y+2\pi), \quad i = 0, \dots l.$$

Then the two-scale Schrödinger operator P defined in (2.11) when applied upon $\tilde{\Psi}^\varepsilon$ gives

$$P(\tilde{\Psi}^\varepsilon) = (c_0 + c_1\varepsilon + c_2\varepsilon^2 + \cdots + c_{l+2}\varepsilon^{l+2})e^{i\Phi/\varepsilon},$$

where by a direct calculation,

$$c_0 = [-\partial_t\Phi - \frac{1}{2}(-i\partial_y + \partial_x\Phi)^2 - V(y) - V_e(x)]A_0 =: G(t,x,y)A_0, \tag{3.2}$$

$$c_1 = i\partial_t A_0 + \frac{1}{2}(2\partial_x\cdot\partial_y + 2i\partial_x\Phi\cdot\partial_x + i\partial_x^2\Phi)A_0 + G(t,x,y)A_1 =: iLA_0 + GA_1, \tag{3.3}$$

$$c_j = \partial_x^2 A_{j-2} + iLA_{j-1} + GA_j, \quad j = 2,3,\dots,l+2. \tag{3.4}$$

Here

$$L := \partial_t + (-i\partial_y + \partial_x\Phi)\partial_x + \frac{1}{2}\partial_x^2\Phi.$$

Observe that, when Φ is real valued, (3.1) is a standard ansatz of the geometric optics [**14**]. In the construction of geometric optic solutions it is required that $c_j = 0, j = 0,1,\dots l+2$, which gives PDEs for $\Phi, A_0, \cdots, A_l$. However, Φ may develop finite time singularities at 'caustics' and equations for A_j then become undefined [**14**].

Band structure/Bloch decomposition. The relation $c_0 = 0$ can be rewritten as

$$(\Phi_t + H(\partial_x\Phi, y) + V_e(x))A_0 = 0, \tag{3.5}$$

where $H(k,y)$ with $k = \partial_x\Phi$ is a self-adjoint differential operator, when k is real.

$$H(k,y) = \frac{1}{2}(-i\partial_y + k)^2 + V(y). \tag{3.6}$$

We let z_n be the normalized eigenfunction corresponding to $E_n(k)$:

$$H(k,y)z_n = E_n(k)z_n, \quad \langle z_n, z_n\rangle = 1.$$

From now on we will suppress the index n, since the construction for each band remains the same.

We set the leading amplitude as

$$A_0(t,x,y) = a(t,x)z(k(t,x),y), \tag{3.7}$$

where $k = \partial_x\Phi$, hence (3.5) is satisfied as long as Φ solves the Hamilton-Jacobi equation:

$$F(t,x) := \partial_t\Phi + E(\partial_x\Phi) + V_e(x) = 0. \tag{3.8}$$

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A Bloch decomposition-dased Gaussian beam method. Let $(x,p) = (\tilde{x}(t), p(t))$ be a bicharacteristics of (3.8), then

$$\dot{\tilde{x}} = E'(p), \quad \dot{p} = -V_e'(\tilde{x}). \tag{3.9}$$

From now on, we fix a bi-characteristics $\{(\tilde{x}(t), p(t)), t > 0\}$ with initial data $(x_0, \partial_x S_0(x_0))$ for any $x_0 \in K_0 = supp_x(g(x,y))$. We denote by γ its projection into the (x,t) space.

The idea underlying the Gaussian beam method is to build asymptotic solutions concentrated on a single ray γ so that $\Phi(t, \tilde{x}(t))$ is real and $Im\{\Phi(t,x)\} > 0$ for $x \neq \tilde{x}(t)$. We are going to choose Φ so that $Im(\Phi) \geq cd(x,\gamma)^2$, where $d(x,\gamma)$ is a distance from x to the central ray γ [**38**]. Therefore, instead of solving (3.8) exactly, we only need to have $F(x,t)$ vanish to higher order on γ. For the first order Gaussian beam approximation we choose the phase $\Phi(t,x)$ a quadratic function:

$$\Phi(t,x) = S(t) + p(t)(x - \tilde{x}(t)) + \frac{1}{2}M(t)(x - \tilde{x}(t))^2. \tag{3.10}$$

With this choice we have

$$F(t,x) = \dot{S} + \dot{p}(x-\tilde{x}) - p\dot{\tilde{x}} + \frac{1}{2}\dot{M}(x-\tilde{x})^2 - M(x-\tilde{x})\dot{\tilde{x}} + E(p + M(x-\tilde{x})) + V_e(x). \tag{3.11}$$

We see that $F(t, \tilde{x}(t)) = 0$ gives the evolution equation for S,

$$\dot{S} = pE'(p) - E(p) - V_e(\tilde{x}).$$

It can be verified $\partial_x F(t, \tilde{x}(t)) = 0$ is equivalent to $\dot{p} = -V_e'(\tilde{x})$, which is the second equation in (3.9). From $\partial_x^2 F(t, \tilde{x}(t)) = 0$ we obtain the equation for M:

$$\dot{M} = -E''(p)M^2 - V_e''(\tilde{x}). \tag{3.12}$$

It is clear that we should set initial condition for the phase as

$$S(0) = S_0(x_0), \tag{3.13}$$

where S_0 is a given initial phase in (1.2). Note that equation (3.12) is a nonlinear Ricatti type equation. The important result about M is given in [**14**], proving that global solution for M exists and $Im(M)$ remains positive (positive definite in multi-dimensional setting) for all time t as long as $Im(M(0))$ is positive. Therefore we choose

$$M(0) = \partial_x^2 S_0(x_0) + i, \tag{3.14}$$

which satisfies $Im(M(0)) > 0$ as required in the Gaussian beam approximation.

It follows from our construction that c_0 vanishes up to third order on $\tilde{x}$. In fact,

$$\begin{aligned} c_0 &= G(az(k(t,x),y)) \\ &= a(t,x)F(t,x)z(k(t,x),y) \\ &= \frac{a(t,x)}{3!}\partial_x^3 F(t,x^*)z(k(t,x),y)(x-\tilde{x})^3, \end{aligned} \tag{3.15}$$

where x^* is an intermediate value between x and $\tilde{x}$. A simple calculation gives

$$\partial_x^3 F(t,x^*) = (V_e^{(3)}(x^*) + E^{(3)}(p + M(x^* - \tilde{x}))M^3(t)), \tag{3.16}$$

which is uniformly bounded near the ray $\tilde{x}$ since $V_e \in C_b^5(\mathbb{R})$ and (1.5) holds. Hence c_0 will be bounded by $O(|x-\tilde{x}|^3)$ as long as the amplitude is bounded.

Equation for the amplitude. For the first order Gaussian beam construction, we shall determine the amplitudes so that c_1 vanishes to the first order on γ. Note that

$$c_1 = iLA_0 + GA_1,$$

where

$$G = -(\Phi_t + H(k,y) + V_e(x)) = -F(t,x) + E(k) - H(k,y).$$

On the ray $x = \tilde{x}(t)$, we require that $c_1 = 0$, that is

$$iLA_0 + (E(p) - H(p,y))A_1 = 0.$$

In order for A_1 to exist, it is necessary that

$$\langle LA_0, z\rangle|_{x=\tilde{x}(t)} = 0. \tag{3.17}$$

For $x \neq \tilde{x}(t)$, we have

$$c_1 = iLA_0 - FA_1 + (E(k) - H(k,y))A_1^\top,$$

where $A_1^\top$ contains the orthogonal compliment of z, satisfying $\langle A_1^\top, z\rangle = 0$. We let

$$A_1^\top = i(E(k) - H)^{-1}[\langle LA_0, z\rangle z - L(A_0)]. \tag{3.18}$$

Therefore using (3.17) and Taylor expansion at $\tilde{x}$,

$$c_1 = i\langle LA_0, z\rangle - FA_1 = i\partial_x\langle LA_0, z\rangle(t, x^*)(x - \tilde{x}) - FA_1. \tag{3.19}$$

With further refined calculation, (3.17) and (3.19) yield the following result.

LEMMA 3.1. *For the first order Gaussian beam construction, $a(t,x) = a(t;x_0)$ and satisfies the following evolution equation along the ray $x = \tilde{x}(t)$:*

$$a_t = a\Big(V_e'(\tilde{x})\langle\partial_k z(p,\cdot), z(p,\cdot)\rangle - \frac{1}{2}E''(p)M\Big). \tag{3.20}$$

Moreover, for $x \neq \tilde{x}(t)$ we have

$$c_0 = \frac{a(t;x_0)}{3!}\partial_x^3 F(t,x^*)z(k,y)(x-\tilde{x})^3, \tag{3.21}$$

$$c_1 = -ia\langle\partial_k z(p,\cdot), z(p,\cdot)\rangle(E''(p)M^2 + V_e''(\tilde{x}))(x-\tilde{x}) - F(t,x)A_1, \tag{3.22}$$

$$c_2 = a(t;x_0)M^2\partial_k^2 z(k,y) + iLA_1, \tag{3.23}$$

where $A_1 \in span\{A_1^\top, z\}$.

PROOF. Recall that

$$A_0 = az(k(t,x),y), \quad k(t,x) = p(t) + M(t)(x - \tilde{x}(t))$$

and

$$L = \partial_t + H_k(k,y)\partial_x + \frac{1}{2}\partial_x^2\Phi = \partial_t + H_k(k,y)\partial_x + \frac{1}{2}M.$$

We take $a(t,x) = a(t;x_0)$, and calculate

$$\begin{aligned}\langle L(az), z\rangle &= \partial_t a + \frac{1}{2}aM + a\langle\partial_t z, z\rangle + a\langle H_k\partial_x z, z\rangle \\ &= \partial_t a + a\left(\frac{1}{2}M + k_t\langle\partial_k z, z\rangle + k_x\langle H_k\partial_k z, z\rangle\right).\end{aligned}$$

We observe that the eigenvalue identity $Hz = Ez$ holds for any k, implying

$$H_{kk}z + 2H_k\partial_k z + H\partial_k^2 z = E''(k)z + 2E'\partial_k z + E\partial_k^2 z.$$

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This against z using $H_{kk} = 1$ and $\langle (H - E)\partial_k^2 z, z\rangle = 0$ leads to

$$E''(k) = 1 + 2\langle H_k \partial_k z, z\rangle - 2E'\langle \partial_k z, z\rangle.$$

Hence using $k_x = M$ we have

$$\frac{1}{2}M + k_x\langle H_k\partial_k z, z\rangle = \frac{1}{2}E''(k)M + E'M\langle \partial_k z, z\rangle.$$

Putting together we obtain

$$\langle L(az), z\rangle = \partial_t a + a\left(\frac{1}{2}E''(k)M + (k_t + E'M)\langle \partial_k z, z\rangle\right),$$

where

$$k_t = -V_e'(\tilde{x}) - E'(p)M + \dot{M}(x - \tilde{x}(t)).$$

Thus (3.17) gives the desired amplitude equation. Recalling (3.15) and (3.16) we have (3.21). (3.19) yields

$$c_1 = ia\dot{M}\langle \partial_k z, z\rangle(x - \tilde{x}) - FA_1,$$

which in virtue of (3.12) gives (3.22). From (3.4) it follows that

$$c_2 = \partial_x^2(az) + iLA_1 = a(k_x)^2\partial_k^2 z + iLA_1$$

which gives (3.23). □

Therefore, the system of ODEs for GB components is set up:

$$\begin{cases} \dot{\tilde{x}} = E'(p), \quad \tilde{x}|_{t=0} = x_0, \\ \dot{p} = -V_e'(\tilde{x}), \quad p|_{t=0} = \partial_x S_0(x_0), \\ \dot{S} = pE'(p) - E(p) - V_e(\tilde{x}), \quad S|_{t=0} = S_0(x_0), \\ \dot{M} = -E''(p)M^2 - V_e''(\tilde{x}), \quad M|_{t=0} = \partial_x^2 S_0(x_0) + i, \\ \dot{a} = a(V_e'(\tilde{x})\langle \partial_k z(p,\cdot), z(p,\cdot)\rangle - \frac{1}{2}E''(p)M), \quad a|_{t=0} = a(x_0), \end{cases} \tag{3.24}$$

where the initial value for the amplitude $a(t; x_0)$ is taken as

$$a|_{t=0} = a(x_0) = \int_0^{2\pi} g(x,y)\overline{z(\partial_x S_0, y)}dy. \tag{3.25}$$

Remark 3.1. *For the derivation of the equations for the Gaussian beam components for the higher order approximations, we refer the reader to* [**14**].

In order to complete the estimate for c_i, we still need to estimate A_1. The following result will be used later in the estimate of the evolution error.

Lemma 3.2. *For any positive integer m, each eigenvector $z_n(k,y)$ satisfies the following condition:*

$$\sum_{|\beta_1|\le m, |\beta_2|\le 3} \|\partial_k^{\beta_1}\partial_y^{\beta_2} z_n(k,y)\|_{L_y^2} \le Z < \infty. \tag{3.26}$$

Proof. For every fixed k, let $(z(k,y), E(k))$ be an eigen-pair that satisfies the eigenvalue equation (1.4), i.e,

$$H(k,y)z(k,y) = \left(\frac{1}{2}(-i\nabla_y + k)^2 + V(y)\right)z(k,y) = E(k)z(k,y), \quad y \in \Gamma. \tag{3.27}$$

Since $V \in C^2(\Gamma)$ and $E \in L^\infty$, by the elliptic regularity theory [**17**, Theorem 6.19], $z(k,y) \in C^3(\Gamma)$ in y variable, which gives (3.26) for $m = 0$.

We next prove (3.26) by induction. We assume that $\partial_k^\beta z \in C^3(\Gamma)$ for $|\beta| \le l-1$ with $1 \le l \le m-1$. Note that $\partial_k^\alpha H = 0$ for any α with $|\alpha| \ge 3$, then differentiation of (3.27) to higher order, using the general Leibnitz rule, gives

$$(H(k,y)-E(k))\partial_k^\beta z = \sum_{\alpha<\beta} \begin{pmatrix} \beta \\ \alpha \end{pmatrix} (\partial_k^{\beta-\alpha} E(k))(\partial_k^\alpha z) - \sum_{\alpha<\beta, |\alpha|\ge|\beta|-2} \begin{pmatrix} \beta \\ \alpha \end{pmatrix} (\partial_k^{\beta-\alpha} H(k,y))(\partial_k^\alpha z). \tag{3.28}$$

The same elliptic regularity theory when applied to (3.28) yields

$$\partial_k^\beta z \in C^3(\Gamma), \quad |\beta| = l.$$

Here the needed $\partial_k^{\beta-\alpha} E \in L^\infty$ is ensured again by assumption (1.5). The proof of (3.26) is complete. □

LEMMA 3.3. *With the eigenvector $z(k,y)$ satisfying (3.26), we have that for $\alpha = 0, 1$,*

$$\sup_{t,x_0} \int_0^{2\pi} |L^\alpha A_1|^2 dy \le CZ(1+Z+Z^2), \tag{3.29}$$

where C depends on the spectral gap $\Delta E = \min_{i\ne j} |E_i - E_j| > 0$ and the Gaussian beam components.

PROOF. Since A_1 is a linear combination of $A_1^\top$ and z, we will prove (3.29) for $A_1^\top$ only. Set

$$B := i(LA_0 - \langle LA_0, z\rangle z),$$

we have

$$A_1^\top = (H-E)^{-1} B. \tag{3.30}$$

We proceed in two steps:

Step 1. Estimate of $LA_1^\top$ in terms of B.

A careful calculation gives that

$$(H-E)LA_1^\top = LB - k_t(H_k - E_k)A_1^\top - k_x H_k(H_k-E_k)A_1^\top + iV'(y)\partial_x A_1^\top. \tag{3.31}$$

In fact, applying L to (3.30) gives

$$(H_k-E_k)k_t A_1^\top + (H-E)\partial_t A_1^\top + H_k\partial_x[(H-E)A_1^\top] + \frac{1}{2}k_x(H-E)A_1^\top = LB.$$

Note that

$$\partial_x[(H-E)A_1] = (H_k-E_k)k_x A_1 + (H-E)\partial_x A_1.$$

Using the definition of operators H and H_k we also have

$$H_k(H-E) = (H-E)H_k - iV'(y).$$

These together verify (3.31).

From (3.31) it follows that

$$\|LA_1^\top\|_{L_y^2} \le \frac{C}{\Delta E}\left(\|LB\|_{L_y^2} + \sum_{j=0}^{2} \|\partial_y^j A_1^\top\|_{L_y^2} + \|\partial_x A_1^\top\|_{L_y^2}\right), \tag{3.32}$$

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here C depends on k_t, k_x, E_k and $V'(y)$, and we have used the following resolvent estimate,

$$\|(H-E)^{-1}\|_{L^2} \leq \frac{1}{\Delta E},$$

where the domain of the operator $(H-E)^{-1}$ is restricted to the orthogonal complement of the eigenvector z. Next we estimate the right hand of (3.32) in terms of B. From here on we use C to denote a generic constant depending on ΔE, k, E, z and their derivatives. We note that

$$LB = B_t + H_k B_x + \frac{1}{2}k_x B = B_t - iB_{xy} + kB_x + \frac{1}{2}k_x B,$$

which yields

$$\|LB\|_{L^2_y} \leq C(\|B\|_{L^2_y} + \|B_t\|_{L^2_y} + \|B_x\|_{L^2_y} + \|B_{xy}\|_{L^2_y}).$$

In the rest of this proof, we shall use $\|\cdot\|$ to denote $\|\cdot\|_{L^2_y}$.

From (3.30) it follows that

$$\begin{aligned} B_y &= (H-E)A_{1y} - iV'(y)A_1, \\ B_{yy} &= (H-E)A_{1yy} - 2iV'(y)A_{1y} - iV''(y)A_1, \\ B_x &= (H-E)A_{1x} + k_x(H_k - E_k)A_1. \end{aligned}$$

Again from (3.30) we obtain $\|A_1^\top\| \leq C\|B\|$, which when combined with the above gives

$$\begin{aligned} \|A_{1y}\| &\leq C(\|B\| + \|B_y\|), \\ \|A_{1yy}\| &\leq C\left(\|B_{yy}\| + \|A_{1y}\| + \|A_1\|\right) \leq C\sum_{j=0}^{2}\|\partial_y^j B\|, \\ \|A_{1x}\| &\leq C\left(\|B_x\| + \|A_{1y}\| + \|A_1\|\right) \leq C\left(\|B\| + \|B_y\| + \|B_x\|\right). \end{aligned}$$

Therefore,

$$\|LA_1^\top\| \leq C(\|B\| + \|B_t\| + \|B_x\| + \|B_{xy}\| + \|B_y\| + \|B_{yy}\|). \tag{3.33}$$

Step 2. Estimate of B.

Note that

$$\begin{aligned} B &= L(az) - \langle L(az), z\rangle z \\ &= ak_t(z_k - \langle z_k, z\rangle z) + ak_x(H_k z_k - \langle H_k z_k, z\rangle z) \\ &= ak_t\tilde{f}_1 + ak_x\tilde{f}_2, \end{aligned}$$

where $\tilde{f}_i$ are of the form

$$\tilde{f}(k,y) = f(k,y) - \langle f(k,\cdot), z(k,\cdot)\rangle z(k,y),$$

with $f_1 = z_k$ and $f_2 = H_k z_k = -iz_{ky} + kz_k$. The right hand side of (3.33) is majored by

$$I_1 + I_2 := C\sum_{i=1}^{2}((\|\tilde{f}_i\| + \|\partial_t\tilde{f}_i\| + \|\partial_x\tilde{f}_i\| + \|\partial_{xy}^2\tilde{f}_i\| + \|\partial_y\tilde{f}_i\| + \|\partial_y^2\tilde{f}_i\|).$$

We apply Lemma 3.4 below to bound both I_1 and I_2.

$$\begin{aligned} I_1 &\le C(\|z_k\| + \|z_{kk}\| + \|z_k\|^2 + (1+\|z_k\|)(\|z_{ky}\| + \|z_{kyy})\|) + \|z_{kky}\| \\ &\quad \|z_{kk}\|\|z_y\| + \|z_{ky}\|\|z_k\| + \|z_k\|^2\|z_y\|) \\ &\le CZ(1+Z+Z^2). \end{aligned}$$

Since $f_2 = -iz_{ky} + kf_1$, it suffices to bound I_2 by considering only $f_2 = z_{ky}$. By Lemma 3.4 we have

$$\begin{aligned} I_2 &\le C(\|z_{ky}\| + \|z_{kky}\| + \|z_{ky}\|\|z_k\| \\ &\quad + \|z_{kyy}\| + \|z_{kyyy}\| + \|z_{ky}\|(1+\|z_y\| + \|z_{yy}\|) \\ &\quad + \|z_{kkyy}\| + \|z_{kky}\|\|z_y\| + \|z_{kyy}\|\|z_k\| + \|z_{ky}\|^2 + \|z_{ky}\|\|z_k\|\|z_y\|) \\ &\le CZ(1+Z+Z^2). \end{aligned}$$

These together with (3.33) yield

$$\|LA_1^\top\| \le CZ(1+Z+Z^2).$$

This proves the boundedness of $\|LA_1\|$. □

LEMMA 3.4. *Let $f(k,y)$ be smooth and integrable in y and*

$$\tilde f(k,y) = f(k,y) - \langle f(k,\cdot), z(k,\cdot)\rangle z(k,y). \tag{3.34}$$

Then for $k = k(t,x)$ the following estimates hold:

(1) $\|\tilde f_t, \tilde f_x\| \le C(\|f_k\| + \|f\|\|z_k\|)$,

(2) $\|\partial_y^j \tilde f\| \le \|\partial_y^j f\| + \|f\|\|\partial_y^j z\|, \quad j = 1,2,$

(3) $\|\tilde f_{xy}\| \le C(\|f_{ky}\| + \|f_k\|\|z_y\| + \|f_y\|\|z_k\| + \|f\|\|z_{ky}\| + \|f\|\|z_k\|\|z_y\|)$,

where constant C depends on k_t and k_x, and the norm $\|\cdot\| := \|\cdot\|_{L^2_y}$.

PROOF. By the chain rule,

$$\tilde f_t = k_t f_k - k_t\langle f_k, z\rangle z - \overline{k_t}\langle f, z_k\rangle z - k_t\langle f, z\rangle z_k.$$

Using the Cauchy inequality together with the fact that z is normalized, we obtain

$$\|\tilde f_t\| \le C(\|f_k\| + 2\|f\|\|z_k\|).$$

Same estimate follows for f_x.

For differentiation in y we have

$$\partial_y^j \tilde f = \partial_y^j f - \langle f, z\rangle \partial_y^j z,$$

leading to

$$\|\partial_y^j \tilde f\| \le \|\partial_y^j f\| + \|f\|\|\partial_y^j z\|.$$

Finally,

$$\tilde f_{xy} = k_x f_{ky} - k_x\langle f_k, z\rangle z_y - \overline{k_x}\langle f, z_k\rangle z_y - k_x\langle f, z\rangle z_{ky}.$$

Hence

$$\|\tilde f_{xy}\| \le C(\|f_{ky}\| + \|f_k\|\|z_y\| + \|f\|\|z_k\|\|z_y\| + \|f\|\|z_{ky}\|)$$

which concludes the proof of the lemma. □

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Gaussian beam superposition and residuals. We solve ODE system (3.24) for each band, and obtain a band based Gaussian beam approximation along a given ray:

$$\tilde{\Psi}^{\varepsilon n}_{GB}(t,x,y;x_0) = (a_n(t;x_0)z_n(k_n,y) + \varepsilon A^n_1(t,x,y;x_0))e^{i\Phi_n(t,x;x_0)/\varepsilon}. \tag{3.35}$$

Since the Schrödinger equation is linear, the approximate solution can be generated by a superposition of neighboring Gaussian beams and over all available bands

$$\tilde{\Psi}^{\varepsilon}(t,x,y) = \frac{1}{\sqrt{2\pi\varepsilon}}\int_{K_0}\sum_{n=1}^{N}\tilde{\Psi}^{\varepsilon n}_{GB}(t,x,y,x_0)dx_0, \tag{3.36}$$

where $\frac{1}{\sqrt{2\pi\varepsilon}}$ is a normalized constant chosen to match initial data against the Gaussian profile. Let us use the notation

$$\tilde{\Psi}^{\varepsilon n}(t,x,y) := \frac{1}{\sqrt{2\pi\varepsilon}}\int_{K_0}\tilde{\Psi}^{\varepsilon n}_{GB}(t,x,y;x_0)dx_0, \tag{3.37}$$

then Lemma 3.1 yields the following residual representation:

$$P(\tilde{\Psi}^{\varepsilon n}) = \frac{1}{\sqrt{2\pi\varepsilon}}\int_{K_0}\left(c_{0n}+\varepsilon c_{1n}+\varepsilon^2 c_{2n}\right)e^{i\Phi_n(t,x;x_0)/\varepsilon}dx_0. \tag{3.38}$$

In next two sections we provide proofs of the accuracy results. We start with the initial error estimation.

4. Initial error—proof of Theorem 2.1.

In this section, the unmarked norm $\|\cdot\|$ denotes $\|\cdot\|_{L^2_{x,y}}$- norm unless otherwise specified.

For simplicity of presentation, we only give the one dimensional estimate with $d = 1$. The initial phase can be expressed as

$$\begin{aligned} S_0(x) &= S_0(x_0) + S_0'(x_0)(x-x_0) + S_0''(x_0)\frac{(x-x_0)^2}{2} + R_2^{x_0}[S_0] \\ &= T_2^{x_0}[S_0](x) + R_2^{x_0}[S_0](x), \end{aligned}$$

where

$$R_2^{x_0}[S_0] = \frac{|S_0^{(3)}(\eta(x,x_0))|(x-x_0)^3}{3!}$$

is the remainder of the Taylor expansion. The idea of the proof of Theorem 2.1 is to introduce

$$\Psi^* = \frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}} g(x_0,y)e^{iT_2^{x_0}[S_0](x)/\varepsilon}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0, \tag{4.1}$$

so that

$$\|\tilde{\Psi}_0 - \tilde{\Psi}_0^{\varepsilon}\| \le \|\tilde{\Psi}_0 - \Psi^*\| + \|\Psi^* - \tilde{\Psi}_0^{\varepsilon}\|, \tag{4.2}$$

where the initial condition $\tilde{\Psi}_0 = \tilde{\Psi}(0,x,y)$ defined in (2.1), $\tilde{\Psi}_0^{\varepsilon} = \tilde{\Psi}^{\varepsilon}(0,x,y)$ defined in (2.8) is the Gaussian beam superposition evaluated at $t = 0$,

$$\tilde{\Psi}_0^{\varepsilon} = \frac{1}{\sqrt{2\pi\varepsilon}}\int_{K_0}\sum_{n=1}^{N}(a_n(x_0)z_n(\partial_x\Phi^0(x;x_0),y) + \varepsilon A^n_1(0,x,y;x_0))e^{i\Phi^0(x;x_0)/\varepsilon}dx_0, \tag{4.3}$$

where from (2.9) we have

$$\Phi^0(x,x_0)=T_2^{x_0}[S_0](x)+\frac{i(x-x_0)^2}{2}.$$

The rest of this section is to estimate two terms on the right of (4.2), which will be given in Lemma 4.1 and Lemma 4.2 below, respectively.

LEMMA 4.1. *Let Ψ^* be defined in (4.1), $g(x,y)\in H^1(K_0\times[0,2\pi])$, then*

$$\|\Psi^*-\tilde{\Psi}_0\|\le\Big(\|\partial_x g\|+\sqrt{\frac{5}{12}}\max_{x\in\mathbb{R}}|S_0^{(3)}(x)|\|g\|\Big)\varepsilon^{1/2}.$$

PROOF. Using that

$$\frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0=1,$$

(4.4)

$$\Psi^*-\tilde{\Psi}_0=\frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}}[g(x_0,y)e^{iT_2^{x_0}[S_0](x)/\varepsilon}-g(x,y)e^{iS_0(x)/\varepsilon}]e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0=I+J,$$

where

$$I=\frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}}(g(x_0,y)-g(x,y))e^{iT_2^{x_0}[S_0](x)/\varepsilon}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0,$$
$$J=\frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}}g(x,y)(e^{iT_2^{x_0}[S_0](x)/\varepsilon}-e^{iS_0(x)/\varepsilon})e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0.$$

Our next step is to find estimates for $\|I\|$ and $\|J\|$.

$$\begin{aligned}\|I\|^2&=\frac{1}{2\pi\varepsilon}\Big\|\int_{\mathbb{R}}(g(x_0,y)-g(x,y))|e^{iT_2^{x_0}[S_0](x)/\varepsilon}|e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big\|\\&=\frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big[\int_{\mathbb{R}}(g(x_0,y)-g(x,y))e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big]^2dxdy.\end{aligned}$$

For fixed x, we introduce a new variable $\xi=\dfrac{x-x_0}{\sqrt{2\varepsilon}}$, $\quad dx_0=-\sqrt{2\varepsilon}d\xi$ to obtain

$$\|I\|^2=\frac{1}{\pi}\int_0^{2\pi}\int_{\mathbb{R}}\Big(\int_{\mathbb{R}}|g(x-\sqrt{2\varepsilon}\xi,y)-g(x,y)|e^{-\xi^2}d\xi\Big)^2dxdy.$$

By the Hölder inequality,

$$\begin{aligned}\|I\|^2&\le\frac{1}{\pi}\int_0^{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}|g(x-\sqrt{2\varepsilon}\xi,y)-g(x,y)|^2e^{-\xi^2}d\xi\int_R e^{-\xi^2}d\xi dxdy\\&=\frac{1}{\sqrt{\pi}}\int_0^{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}|g(x-\sqrt{2\varepsilon}\xi,y)-g(x,y)|^2e^{-\xi^2}d\xi dxdy.\end{aligned}$$

Using the mean value theorem for g, we have

$$g(x-\sqrt{2\varepsilon}\xi,y)-g(x,y)=-\partial_x g(x-\eta^*\sqrt{2\varepsilon}\xi,y)\sqrt{2\varepsilon}\xi=-\partial_x g(x-\eta^*(x-x_0),y)\sqrt{2\varepsilon}\xi.$$

Hence,

$$\begin{aligned}\|I\|^2&\le\frac{2\varepsilon}{\sqrt{\pi}}\int_0^{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}|\partial_x g(x-\eta^*(x-x_0),y)|^2dx\xi^2e^{-\xi^2}d\xi dy\\&=\frac{2\varepsilon}{\sqrt{\pi}}\|\partial_x g\|^2\int_{\mathbb{R}}\xi^2e^{-\xi^2}d\xi=\varepsilon\|\partial_x g\|^2.\end{aligned}$$

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Now we turn to the estimation of $\|J\|$:

$$\begin{aligned}\|J\|^2 &= \frac{1}{2\pi\varepsilon}\Big\| \int_{\mathbb{R}} g(x,y)(e^{iT_2^{x_0}[S_0](x)/\varepsilon} - e^{iS_0(x)/\varepsilon})e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big\|^2 \\ &\leq \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big[\int_{\mathbb{R}}|g(x,y)||e^{iS_0(x)/\varepsilon}||e^{-iR_2^{x_0}[S_0](x)/\varepsilon} \\ &\qquad - 1|e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big]^2 dxdy.\end{aligned}$$

Since S_0 is real, $|e^{iS_0(x)/\varepsilon}| = 1$. The above is further bounded by

$$\begin{aligned}\frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big[\int_{\mathbb{R}}|g(x,y)|\Big[\Big(\cos\frac{R_2^{x_0}[S_0](x)}{\varepsilon} - 1\Big)^2 \\ + \sin^2\frac{R_2^{x_0}[S_0](x)}{\varepsilon}\Big]^{1/2}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big]^2 dxdy.\end{aligned}$$

Using a half-angle formula for $\sin x$ and that $|\sin x| \leq |x|$, we obtain:

$$\begin{aligned}\|J\|^2 &\leq \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big[\int_{\mathbb{R}}|g(x,y)|\Big(4\sin^2\frac{R_2^{x_0}[S_0](x)}{2\varepsilon}\Big)^{1/2}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big]^2 dxdy \\ &\leq \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big[\int_{\mathbb{R}}|g(x,y)|\frac{R_2^{x_0}[S_0](x)}{\varepsilon}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big]^2 dxdy.\end{aligned}$$

Using the remainder formula and the Hölder inequality,

$$\begin{aligned}\|J\|^2 \leq \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}|g(x,y)|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0 \\ \times\int_{\mathbb{R}}\frac{(|S_0^{(3)}(\eta)|)^2}{36}\frac{|x-x_0|^6}{\varepsilon^2}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy.\end{aligned}$$

Now, applying the same change of variable as for the term I, $\xi = \dfrac{x-x_0}{\sqrt{2\varepsilon}}$, ($x$ variable is fixed) we get:

$$\begin{aligned}\|J\|^2 &\leq \frac{1}{2\pi\varepsilon}\|g\|^2\frac{(\max|S_0^{(3)}(x)|)^2}{36}\sqrt{2\pi\varepsilon}\int_{\mathbb{R}}8\sqrt{2}\varepsilon^{-2+3+1/2}|\xi|^6e^{-\xi^2}d\xi \\ &\leq \frac{\sqrt{2\pi}\max_{x\in\mathbb{R}}|S_0^{(3)}(x)|^2}{72\pi}\times 8\sqrt{2}\times\frac{15}{8}\sqrt{\pi}\|g\|^2\varepsilon \\ &= \frac{5}{12}\max_{x\in\mathbb{R}}|S_0^{(3)}(x)|^2\|g\|^2\varepsilon.\end{aligned}$$

Hence, summing both parts, we conclude that:

$$\begin{aligned}\|\Psi^* - \tilde{\Psi}_0\| &\leq \|I\| + \|J\| \\ &\leq \Big(\|\partial_x g\| + \sqrt{\frac{5}{12}}\max_{x\in\mathbb{R}}|S_0^{(3)}(x)|\|g\|\Big)\varepsilon^{1/2}.\end{aligned}$$

□

Our next step is to find an estimate for the difference between GB ansatz and Ψ^*.

LEMMA 4.2. *The following estimate holds:*

$$\|\tilde{\Psi}_0^\varepsilon - \Psi^*\| \le C\varepsilon^{1/2},$$

where

$$C = 2\pi \max_{k,1\le n\le N} \|\partial_k z_n(k,y)\|^2_{L^\infty_y} \int_{K_0} \Big|\sum_{n=1}^N a_n(x_0)\Big|^2 (S_0''^2(x_0)+1)dx_0,$$

can be computed from the initial data.

PROOF. According to our construction,

$$\begin{aligned}\|\tilde{\Psi}_0^\varepsilon - \Psi^*\|^2 &= \Big\|\tilde{\Psi}_0^\varepsilon - \frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}} g(x_0,y)e^{iT_2^{x_0}[S_0](x)/\varepsilon}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big\|^2\\ &= \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big|\int_{K_0}\sum_{n=1}^N (a_n(x_0)(z_n(\partial_x\Phi^0(x,x_0),y) - z_n(\partial_x S_0(x_0),y))\\ &\quad + \varepsilon A_1^n(0,x,y;x_0))e^{\frac{i\Phi^0(x,x_0)}{\varepsilon}}dx_0\Big|^2 dxdy.\end{aligned}$$

Then, putting the absolute value sign inside the integral over K_0, we observe that

$$\begin{aligned}\|\tilde{\Psi}_0^\varepsilon - \Psi^*\|^2 \le \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\Big[\int_{K_0}\Big|\sum_{n=1}^N (a_n(x_0)(z_n(\partial_x\Phi^0(x,x_0),y) - z_n(\partial_x S_0(x_0),y))\\ + \varepsilon A_1^n(0,x,y;x_0))\Big|e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\Big]^2 dxdy.\end{aligned}$$

By the Hölder inequality,

$$\begin{aligned}\|\tilde{\Psi}_0^\varepsilon - \Psi^*\|^2 &\le \frac{1}{2\pi\varepsilon}\int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\Big|\sum_{n=1}^N (a_n(x_0)(z_n(\partial_x\Phi^0(x,x_0),y) - z_n(\partial_x S_0(x_0),y))\\ &\quad + \varepsilon A_1^n(0,x,y;x_0))\Big|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0\int_{K_0}e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy\\ &= \frac{1}{\sqrt{2\pi\varepsilon}}\int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\Big|\sum_{n=1}^N (a_n(x_0)(z_n(\partial_x\Phi^0(x,x_0),y)\\ &\quad - z_n(\partial_x S_0(x_0),y)) + \varepsilon A_1^n(0,x,y;x_0))\Big|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy.\end{aligned}$$

Using that

$$\begin{aligned}z_n(\partial_x\Phi^0(x,x_0),y) - z_n(\partial_x S_0(x_0),y) &= z_n(S_0'(x_0) + (S_0''(x_0)+i)(x-x_0)\\ &\quad - z_n(S_0'(x_0),y)\\ &= \partial_k z_n(\eta_n(x,x_0),y)(S_0''(x_0)+i)(x-x_0),\end{aligned}$$

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we obtain:

$$\begin{aligned}\|\tilde{\Psi}_0^\varepsilon - \Psi^*\|^2 &\le \frac{1}{\sqrt{2\pi\varepsilon}}\int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\Big|\sum_{n=1}^{N}(a_n(x_0)\partial_k z_n(\eta_n(x,x_0),y)(S_0''(x_0)+i)\\ &\quad\cdot(x-x_0)+\varepsilon A_1^n(0,x,y;x_0))\Big|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy\\ &\le \frac{2}{\sqrt{2\pi\varepsilon}}\Big(\int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\Big|\sum_{n=1}^{N}(a_n(x_0)\partial_k z_n(\eta_n(x,x_0),y)(S_0''(x_0)+i)(x-x_0)\Big|^2\\ &\quad\cdot e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy+\varepsilon^2\int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\Big|\sum_{n=1}^{N}A_1^n(0,x,y;x_0))\Big|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy\Big)\\ &= I_1+I_2.\end{aligned}$$

Switching the order of integration and applying the change of variables for fixed x_0,

$$\xi=\frac{x-x_0}{\sqrt{2\varepsilon}},\quad dx=\sqrt{2\varepsilon}d\xi$$

together with the fact that $S_0''(x_0)$ is real,

$$\begin{aligned}I_1 &\le \frac{1}{\sqrt{2\pi\varepsilon}}\int_0^{2\pi}\int_{K_0}\int_{\mathbb{R}}\Big|\sum_{n=1}^{N}a_n(x_0)\partial_k z_n(\eta_n(\xi,x_0),y)(S_0''(x_0)+i)\Big|^2\\ &\quad\cdot 2\varepsilon\xi^2 e^{-\xi^2}\sqrt{2\varepsilon}d\xi dx_0dy\\ &\le \frac{2\varepsilon}{\sqrt{\pi}}\max_{k,1\le n\le N}\|\partial_k z_n(k,y)\|^2_{L_y^\infty}\\ &\quad\cdot\int_{\mathbb{R}}\xi^2 e^{-\xi^2}d\xi\int_0^{2\pi}\int_{K_0}\Big|\sum_{n=1}^{N}a_n(x_0)\Big|^2(S_0''^2(x_0)+1)dx_0dy\\ &\le 2\pi\varepsilon\max_{k,1\le n\le N}\|\partial_k z_n(k,y)\|^2_{L_y^\infty}\int_{K_0}\Big|\sum_{n=1}^{N}a_n(x_0)\Big|^2(S_0''^2(x_0)+1)dx_0.\end{aligned}$$

Since $N<\infty$ is finite, the right hand side is bounded by $C\varepsilon$ where constant C depends on the initial data.

As for I_2,

$$I_2=\frac{\varepsilon^{\frac{3}{2}}}{\sqrt{2\pi}}\int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\Big|\sum_{n=1}^{N}A_1^n(0,x,y;x_0))\Big|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}}dx_0dxdy,$$

we use the definition of A_1 in (3.18), where we use that $(H(k,y)-E(k))^{-1}$ is bounded operator (moreover, it is compact), hence A_1 is bounded. Also, the same change of variables as in the case of I_1 estimate will produce the additional rate of convergence.

Hence,

$$I_2\le C\varepsilon^2$$

and may be neglected since its order of convergence is higher than for I_1. □

Using the triangle inequality, we thus get the estimate for the initial error:

$$\|\tilde{\Psi}_0-\tilde{\Psi}_0^\varepsilon\|\le\|\tilde{\Psi}_0-\Psi^*\|+\|\Psi^*-\tilde{\Psi}_0^\varepsilon\|\le C\varepsilon^{1/2}.$$

5. Evolution error—proof of Theorem 2.2

We prove Theorem 2.2 in several steps, in one dimensional setting; an extension to multi-dimensions will be given in next section. Taking advantage of the band structure of the asymptotic construction and the linearity of the Schrödinger operator, we rewrite

$$P(\tilde{\Psi}^\varepsilon) = P\Big(\sum_{n=1}^N \tilde{\Psi}^{\varepsilon n}\Big) = \sum_{n=1}^N P(\tilde{\Psi}^{\varepsilon n}),$$

where $\tilde{\Psi}^{\varepsilon n}$ is defined in (3.37). By the Minkowski inequality,

$$\|P(\tilde{\Psi}^\varepsilon)\| \le \sum_{n=1}^N \|P(\tilde{\Psi}^{\varepsilon n})\|.$$

Using residual representation of $P(\tilde{\Psi}^{\varepsilon,n})$ from (3.38) in section 3, we have

$$P(\tilde{\Psi}^{\varepsilon n}) = \sum_{j=0}^2 I_{jn},$$

where

$$I_{jn} = \frac{\varepsilon^{j-\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}} \int_{K_0} G_{jn}(t,x;x_0,y)(x-\tilde{x}_n(t;x_0))^{(3-2j)_+} e^{i\Phi_n(t,x;x_0)/\varepsilon} dx_0, \tag{5.1}$$

where

$$G_{0n}(t,x;x_0,y) = \frac{1}{3!} a_n(t;x_0)\partial_x^3 F_n(t,x^*) z_n(k_n,y), \tag{5.2}$$

$$G_{1n}(t,x;x_0) = (ia\langle \partial_k z_n, z_n\rangle \dot{M} - \frac{1}{3!}\partial_x^3 F_n(t,x^*) A_{1n}(x-\tilde{x}_n)^2). \tag{5.3}$$

$$G_{2n}(t,x;x_0,y) = a_n(t;x_0) M_n^2 \partial_k^2 z_n(k_n,y) + iLA_{1n}. \tag{5.4}$$

Let $'$ denote quantities defined on the ray emanating from x_0' such as $\tilde{x}_n', c_{jn}'$ and Φ_n'.

From Lemma 3.1 and Lemma 3.3 it follows the following bound:

$$\int_0^{2\pi} |G_{jn}\overline{G_{jn}'}| dy \le C_1. \tag{5.5}$$

Here we note that G_{1n} contains a term involving $(x-\tilde{x}_n)^2$ which becomes unbounded when x is far away from the ray $\tilde{x}_n$. In such case, the Gaussian beam factor $e^{-\delta|x-\tilde{x}_n|^2/\varepsilon}$ needs to be taken into account.

We compute the L^2 norm of I_{jn} by

$$\begin{aligned}\|I_{jn}\|^2 &= \int_0^{2\pi}\int_{\mathbb{R}} I_{jn}(t,x;x_0,y)\cdot \overline{I_{jn}(t,x;x_0',y)} dxdy \\ &= \int_0^{2\pi}\int_{\mathbb{R}}\int_{K_0}\int_{K_0} J_{jn}(x,y,x_0,x_0') dx_0 dx_0' dxdy,\end{aligned}$$

where

$$J_{jn}(x,y,x_0,x_0') = \frac{\varepsilon^{2j-1}}{2\pi} G_{jn}\overline{G_{jn}'}(x-\tilde{x}_n)^{(3-2j)_+}(x-\tilde{x}_n')^{(3-2j)_+} e^{i\psi_n/\varepsilon} \tag{5.6}$$

with

$$\psi_n(t,x,x_0,x_0') = \Phi_n(t,x;x_0) - \overline{\Phi_n'(t,x;x_0')}. \tag{5.7}$$

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Let $\rho_j(x, x_0, x_0') \in C^\infty$ be a partition of unity such that

$$\rho_2 = \begin{cases} 1, & |x-\tilde{x}_n| \le \eta \cap |x-\tilde{x}_n'| \le \eta, \\ 0, & |x-\tilde{x}_n| \ge 2\eta \cup |x-\tilde{x}_n'| \ge 2\eta, \end{cases} \tag{5.8}$$

and $\rho_1 + \rho_2 = 1$. Moreover, let

$$J_{jn}^1 = \rho_1 J_{jn}(x, y, x_0, x_0'), \qquad J_{jn}^2 = \rho_2 J_{jn}(x, y, x_0, x_0'),$$

so that $J_{jn}(x, y, x_0, x_0') = J_{jn}^1 + J_{jn}^2$.

The rest of this section is to establish the following

$$\left| \int_0^{2\pi} \int_{\mathbb{R}} \int_{K_0} \int_{K_0} J_{jn}^i dx_0 dx_0' dx dy \right| \le C\varepsilon^3 \tag{5.9}$$

for $i = 1, 2$. With this estimate we have $\|I_{jn}\| \le C\varepsilon^{\frac{3}{2}}$, leading to the desired estimate. Since for $i = 2$ we already have the needed convergence rate, the following proof will be concerned with $i = 0$ or $i = 1$ cases.

5.0.1. *Estimate of* J_{jn}^1. Using that $\Im\psi_n = \Im\Phi_n + \Im\Phi_n' \ge \delta(|x-\tilde{x}_n|^2 + |x-\tilde{x}_n'|^2)$ and the definition of ρ_1, in J_{jn}^1 either $|x-\tilde{x}_n(t;x_0)|$ or $|x-\tilde{x}_n(t;x_0')|$ is greater than 2η, hence

$$\int_0^{2\pi} |J_{jn}^1| dy \le C e^{-\frac{\delta}{2\varepsilon}|x-\tilde{x}_n|^2} e^{-\frac{2\eta^2\delta}{\varepsilon}},$$

we thus obtain an exponential decay

$$\left| \int_0^{2\pi} \int_{\mathbb{R}} \int_{K_0} \int_{K_0} J_{jn}^1 dx_0 dx_0' dx dy \right| \le C\Big(\frac{2\pi\varepsilon}{\delta}\Big)^{\frac{1}{2}} |K_0|^2 e^{-\frac{2\eta^2\delta}{\varepsilon}} \le C\varepsilon^s \quad \forall s.$$

5.0.2. *Estimation of* J_{jn}^2. Using the estimate

$$s^p e^{-as^2} \le \Big(\frac{p}{e}\Big)^{p/2} a^{-p/2} e^{-as^2/2},$$

with $s = |x-\tilde{x}_n|$ or $s = |x-\tilde{x}_n'|$, $p = 3, 1, \text{or } 0$, $a = \frac{\delta}{2\varepsilon}$, we have

$$\int_0^{2\pi} |J_{jn}^2| dy \le C C_2 \varepsilon^2 e^{-\frac{\delta}{2\varepsilon}(|x-\tilde{x}_n|^2 + |x-\tilde{x}_n'|^2)},$$

where

$$C_2 \le \frac{1}{2\pi}\left(\frac{6}{e\delta}\right)^{3/2}.$$

Next we note that

$$\begin{aligned} |x-\tilde{x}_n(t;x_0)|^2 + |x-\tilde{x}_n(t;x_0')|^2 = 2\Big|x - \frac{\tilde{x}_n(t;x_0) + \tilde{x}_n(t;x_0')}{2}\Big|^2 \\ + \frac{1}{2}|\tilde{x}_n(t;x_0) - \tilde{x}_n(t;x_0')|^2, \end{aligned} \tag{5.10}$$

with which we have

$$\int_0^{2\pi} \int_{\mathbb{R}} |J_{jn}^2| dx dy \le C\varepsilon^2 \int_{\mathbb{R}} e^{-\frac{\delta}{\varepsilon}x^2} dx e^{-\frac{\delta}{4\varepsilon}|\tilde{x}_n(t;x_0) - \tilde{x}_n(t;x_0')|^2}.$$

Hence,

$$\left| \int_0^{2\pi} \int_{\mathbb{R}} \int_{K_0} \int_{K_0} J_{jn}^2 dx_0 dx_0' dx dy \right| \le C\varepsilon^{\frac{5}{2}} \int_{K_0} \int_{K_0} e^{-\frac{\delta}{4\varepsilon}|\tilde{x}_n(t;x_0) - \tilde{x}_n(t;x_0')|^2} dx_0 dx_0'. \tag{5.11}$$

In order to obtain (5.9), we need to recover an extra $\varepsilon^{\frac{1}{2}}$ from the integral on the right hand side, which is difficult when $|\tilde{x}_n(t;x_0)-\tilde{x}_n(t;x_0')|$ is small.

Following [**31**], we split the set $K_0\times K_0$ into

$$D_1(t,\theta)=\Big\{(x_0,x_0'):|\tilde{x}_n(t,x_0)-\tilde{x}_n(t,x_0')|\geq\theta|x_0-x_0'|\Big\},$$

which corresponds to the non-caustic region of the solution, and the set associated with the caustic region

$$D_2(t,\theta)=\Big\{(x_0,x_0'):|\tilde{x}_n(t,x_0)-\tilde{x}_n(t,x_0')|<\theta|x_0-x_0'|\Big\}.$$

For the former we have

$$\int_{D_1}e^{-\frac{\delta}{4\varepsilon}|\tilde{x}_n(t;x_0)-\tilde{x}_n(t;x_0')|^2}dx_0dx_0'\leq\int_{D_1}e^{-\frac{\delta\theta^2}{4\varepsilon}|x_0-x_0'|^2}dx_0dx_0'.$$

Letting $\Lambda=\sup_{x_0,x_0'\in K_0}|x_0-x_0'|<\infty$ be the diameter of K_0, we continue to estimate the above D_1-integral

$$\int_{D_1}e^{-\frac{\delta\theta^2}{4\varepsilon}|x_0-x_0'|^2}dx_0dx_0'\leq C\int_0^{\Lambda}e^{-\frac{\delta\theta^2}{4\varepsilon}\tau^2}d\tau\leq C\varepsilon^{1/2},$$

which concludes the estimate of J_{jn}^2 when restricted on D_1 in (5.11).

To estimate J_{jn}^2 restricted on D_2, we need the following result on phase estimate.

LEMMA 5.1. ***(Phase estimate)*** *For $(x_0,x_0')\in D_2$, it holds*

$$|\partial_x\psi_n(t,x,x_0,x_0')|\geq C(\theta,\eta)|x_0-x_0'|,$$

where $C(\theta,\eta)$ is independent of x and positive if θ and η are sufficiently small.

The proof of this result is due to [**31**], where the non-squeezing lemma is crucial. Since all requirements for the non-squeezing argument are satisfied by the construction of Gaussian beam solutions in present work, we therefore omit details of the proof.

To continue, we note that the phase estimate ensures that for $(x_0,x_0')\in D_2$, $x_0\neq x_0'$, $\partial_x\psi_n(t,x,x_0,x_0')\neq 0$. Therefore, in order to estimate $J_{jn}^2|_{D_2}$ we shall use the following non-stationary phase lemma.

LEMMA 5.2. ***(Non-stationary phase lemma)*** *Suppose that $u(x,\xi)\in C_0^\infty(\Omega\times Z)$ where Ω and Z are compact sets and $\psi(x;\xi)\in C^\infty(O)$ for some open neighborhood O of $\Omega\times Z$. If $\partial_x\psi$ never vanishes in O, then for any $K=0,1,\ldots,$*

$$\Big|\int_\Omega u(x;\xi)e^{i\psi(x;\xi)/\varepsilon}dx\Big|\leq C_K\varepsilon^K\sum_{\alpha=1}^K\int_\Omega\frac{|\partial_x^\alpha u(x;\xi)|}{|\partial_x\psi(x;\xi)|^{2K-\alpha}}e^{-\Im\psi(x;\xi)/\varepsilon}dx,$$

where C_K is a constant independent of ξ.

Using the non-stationary lemma, we obtain for $(x_0,x_0')\in D_2$,

$$\Big|\int_0^{2\pi}\int_{\mathbb{R}}J_{jn}^2dxdy\Big|=\frac{C_K\varepsilon^{K+2j-1}}{2\pi}\times\int_0^{2\pi}\int_{\mathbb{R}}\sum_{\alpha=1}^K\frac{|\partial_x^\alpha[\rho_1G_{jn}\overline{G_{jn}'}(x-\tilde{x}_n)^{3-2j}(x-\tilde{x}_n')^{3-2j}]|}{|\partial_x\psi_n(t,x;x_0,x_0')|^{2K-\alpha}}e^{-\Im\psi_n(x;\xi)/\varepsilon}dxdy.$$

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By Leibniz's rule,

$$\begin{aligned}\partial_x^\alpha[\rho_1 G_{jn}\overline{G'_{jn}}(x-\tilde{x}_n)^{3-2j}(x-\tilde{x}'_n)^{3-2j}] &= \sum_{\alpha_1+\alpha_2=\alpha}(\partial_x^{\alpha_1}[\rho_1 G_{jn}\overline{G'_{jn}}]\\ &+ \partial_x^{\alpha_2}[(x-\tilde{x}_n)^{3-2j}(x-\tilde{x}'_n)^{3-2j}]).\end{aligned}$$

Here we take a detailed look at the term $\Big|\int_0^{2\pi}\partial_x^{\alpha_1}[\rho_1 G_{jn}\overline{G'_{jn}}]dy\Big|$, for each case when $j=0,1$. For $j=0$, we have

$$\begin{aligned}\Big|\int_0^{2\pi}\partial_x^{\alpha_1}[\rho_1 G_{0n}\overline{G'_{0n}}]dy\Big| &= \Big|\int_0^{2\pi} a_n\overline{a'_n}\partial_x^{\alpha_1}(\rho_1\partial_x^3 F_n z_n\overline{\partial_x^3 F'_n z'_n})dy\Big|\\ &= \Big|\sum_{\alpha_{11}+\alpha_{12}=\alpha_1} a_n\overline{a'_n}\partial_x^{\alpha_{11}}[\rho_1\partial_x^3 F_n\overline{\partial_x^3 F'_n}]\cdot\int_0^{2\pi}\partial_x^{\alpha_{12}}[z_n\overline{z'}_n]dy\Big|\\ &\le |a_n|^2|M_n|^{\alpha_{12}}\cdot\sum_{\alpha_{11}+\alpha_{12}=\alpha_1}\partial_x^{\alpha_{11}}[\rho_1\partial_x^3 F_n\overline{\partial_x^3 F'_n}]\cdot\int_0^{2\pi}\partial_k^{\alpha_{12}}[z_n\overline{z'}_n]dy\Big|\\ &\le CZ^2 := C_2.\end{aligned}$$

For $j=1$, we notice that G_{1n} does not depend on y,

$$\begin{aligned}\Big|\partial_x^{\alpha_1}[\rho_1 G_{1n}\overline{G'_{1n}}]\Big| &\sim \Big|a_n\overline{a'_n}\partial_x^{\alpha_1}(\rho_1\dot{M}_n\langle\partial_k z_n, z_n\rangle\overline{\dot{M}'_n\langle\partial_k z'_n, z'_n\rangle})\Big|\\ &= \Big|\sum_{\alpha_{11}+\alpha_{12}=\alpha_1} a_n\overline{a'_n}\partial_x^{\alpha_{11}}[\rho_1\dot{M}_n\overline{\dot{M}'_n}]\cdot\partial_x^{\alpha_{12}}[\langle\partial_k z_n, z_n\rangle\overline{\langle\partial_k z'_n, z_n\rangle}]\Big|\\ &\le |a_n|^2|M_n|^{\alpha_{12}}\cdot\sum_{\alpha_{11}+\alpha_{12}=\alpha_1}|\partial_x^{\alpha_{11}}[\rho_1\dot{M}_n\overline{\dot{M}'_n}]\partial_k^{\alpha_{12}}[\langle\partial_k z_n, z_n\rangle\overline{\langle\partial_k z'_n, z_n\rangle}]|\\ &\le CZ^2 := C_2.\end{aligned}$$

Here we used the fact that indices α_{11} and α_{12} are not greater than 2 and j is either 0 or 1, which is consistent with the boundedness requirement in (3.26).

Going further,

$$\begin{aligned}\partial_x^{\alpha_2}[(x-\tilde{x}_n)^{3-2j}(x-\tilde{x}'_n)^{3-2j}] \le & C\sum_{\alpha_{21}+\alpha_{22}=\alpha_2}(x-\tilde{x}_n)^{3-2j-\alpha_{21}}\\ &\cdot(x-\tilde{x}'_n)^{3-2j-\alpha_{22}},\end{aligned}$$

we have

$$\begin{aligned}&\int_0^{2\pi}\int_{\mathbb{R}}|\partial_x^{\alpha_1}[\rho_1 G_{jn}\overline{G'_{jn}}]\partial_x^{\alpha_2}[(x-\tilde{x}_n)^{3-2j}(x-\tilde{x}'_n)^{3-2j}]|e^{-\Im\psi_n/\varepsilon}dxdy\\ &\le C\sum_{\alpha_{21}+\alpha_{22}=\alpha_2}\int_{\mathbb{R}}|x-\tilde{x}_n|^{3-2j-\alpha_{21}}|x-\tilde{x}'_n|^{3-2j-\alpha_{22}}e^{-\Im\psi_n/\varepsilon}dx\\ &\le C\varepsilon^{\frac{-\alpha_2}{2}+3-2j}\int_{\mathbb{R}}e^{-\frac{\delta}{\varepsilon}(|x-\tilde{x}_n|^2+|x-\tilde{x}'_n|^2)}dx\\ &\le C\left(\frac{\pi}{\delta}\right)^{1/2}\varepsilon^{\frac{1-\alpha_2}{2}+3-2j}e^{-\frac{\delta}{2\varepsilon}|\tilde{x}_n-\tilde{x}'_n|^2},\end{aligned}$$

where (5.10) has been used. Hence,

$$\left|\int_0^{2\pi}\int_{\mathbb{R}}\int_{D_2} J_{jn}^2 dx_0 dx_0' dx dy\right| \le \int_{D_2} e^{-\frac{\delta}{2\varepsilon}|\tilde{x}-\tilde{x}'|^2}\sum_{\alpha=1}^{K}\frac{\varepsilon^{\frac{\alpha}{2}+2j-1}}{\inf|\partial_x\psi_n/\sqrt{\varepsilon}|^{2K-\alpha}}$$
$$\cdot\sum_{\alpha_1+\alpha_2=\alpha} C\varepsilon^{\frac{1-\alpha_2}{2}+3-2j}dx_0dx_0'$$
$$\le C\varepsilon^{\frac{5}{2}}\int_{D_2} e^{-\frac{\delta}{2\varepsilon}|\tilde{x}_n-\tilde{x}_n'|^2}\sum_{\alpha=1}^{K}\frac{1}{\inf|\partial_x\psi_n/\sqrt{\varepsilon}|^{2K-\alpha}}dx_0dx_0'.$$

The last estimate together with (5.11) yields:

$$\begin{aligned}
\left|\int J_{jn}^2 1_{D_2}\right| &\le C\varepsilon^{\frac{5}{2}}\int_{D_2} e^{-\frac{\delta}{2\varepsilon}|\tilde{x}_n-\tilde{x}_n'|^2}\min\Big[1,\sum_{\alpha=1}^{K}\frac{1}{\inf|\partial_x\psi_n/\sqrt{\varepsilon}|^{2K-\alpha}}\Big]dx_0dx_0'\\
&\le C\varepsilon^{\frac{5}{2}}\int_{D_2} e^{-\frac{\delta}{2\varepsilon}|\tilde{x}_n-\tilde{x}_n'|^2}\sum_{\alpha=1}^{K}\min\Big[1,\frac{1}{\inf|\partial_x\psi_n/\sqrt{\varepsilon}|^{2K-\alpha}}\Big]dx_0dx_0'\\
&\le C\varepsilon^{\frac{5}{2}}\int_{K_0}\int_{K_0} e^{-\frac{\delta}{2\varepsilon}|\tilde{x}_n-\tilde{x}_n'|^2}\sum_{\alpha=1}^{K}\frac{1}{1+\inf|\partial_x\psi_n/\sqrt{\varepsilon}|^{2K-\alpha}}dx_0dx_0'\\
&\le C\varepsilon^{\frac{5}{2}}\int_{K_0}\int_{K_0}\sum_{\alpha=1}^{K}\frac{1}{1+(C(\theta,\eta)|x_0-x_0'|/\sqrt{\varepsilon})^{2K-\alpha}}dx_0dx_0'.
\end{aligned}$$

Taking $K=2$ and changing variable $\xi=\dfrac{x_0-x_0'}{\sqrt{\varepsilon}}$, we compute

$$\left|\int J_{jn}^2 1_{D_2}\right| \le C\varepsilon^{\frac{5}{2}}\int_{K_0\times K_0}\frac{1}{1+(|x_0-x_0'|/\sqrt{\varepsilon})^K}dx_0dx_0'$$
$$\le C\varepsilon^3\int_0^{\infty}\frac{1}{1+\xi^K}d\xi=\frac{\pi}{2}C\varepsilon^3,$$

which gives (5.9) when restricted to the caustic region.

Putting all together we complete the proof of (5.9), hence Theorem 2.2.

6. Extensions

The extension of the one-dimensional results to multidimensional case is straightforward. We still have the two-scale formulation,

$$i\varepsilon\frac{\partial\tilde{\Psi}}{\partial t}=-\frac{1}{2}(\varepsilon\nabla_x+\nabla_y)^2\tilde{\Psi}+V(\frac{x}{\varepsilon})\tilde{\Psi}+V_e(x)\tilde{\Psi},\quad x\in\mathbb{R}^d, \tag{6.1}$$

$$\Psi(0,x,y)=g(x,y)e^{iS_0(x)/\varepsilon},\quad x\in K_0\subset\mathbb{R}^d,\quad y\in[0,2\pi]^d. \tag{6.2}$$

The Gaussian beam construction of the phase will have the following form:

$$\Phi(t,x;x_0)=S(t;x_0)+p(t;x_0)\cdot(x-\tilde{x}(t;x_0))+\frac{1}{2}(x-\tilde{x}(t;x_0))^{\top}\cdot M(x-\tilde{x}(t;x_0)). \tag{6.3}$$

Following the procedure of the Gaussian beam construction in section 3, we only check possible different formulations in the multidimensional setting. For instance, equation (3.4) will take a form:

$$c_j=\Delta_x A_{j-2}+iLA_{j-1}+GA_j,\quad j=2,3,\dots,l+2,$$

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where L reads

$$L = \partial_t + (-i\nabla_y + \nabla_x\Phi)\cdot\nabla_x + \frac{1}{2}\Delta_x\Phi.$$

The evolution equations for the Gaussian beam phase components:

$$\begin{cases} \dot{\tilde{x}} = \nabla_k E(p), \quad \tilde{x}|_{t=0} = x_0, \\ \dot{p} = -\nabla_x V_e(\tilde{x}), \quad p|_{t=0} = \nabla_x S(x_0), \\ \dot{S} = p\cdot\nabla_k E(p) - E(p) - V_e(\tilde{x}), \quad S|_{t=0} = S_0(x_0), \\ \dot{M} = -M\nabla_k^2 E(p) M - \nabla_x^2 V_e(\tilde{x}), \quad M|_{t=0} = \nabla_x^2 S_0(x_0) + iI. \end{cases} \tag{6.4}$$

An equation for the amplitude can be derived from (3.19), however because of the matrix M, it has more sophisticated form than in 1- dimensional case:

$$\dot{a} = a(\langle(\nabla_k z\cdot(\nabla_x V_e(\tilde{x}) + M\nabla_k E(p)), z\rangle - \langle(-i\nabla_y + p)\cdot M\nabla_k z, z\rangle - \frac{1}{2}Tr(M)). \tag{6.5}$$

One can easily verify that the amplitude equation for $d = 1$ follows from (6.5).

The superposition formula (3.37) for the approximate solution is:

$$\tilde{\Psi}^\varepsilon(t,x,y) = \frac{1}{(2\pi\varepsilon)^{d/2}}\int_{K_0}\tilde{\Psi}^\varepsilon_{GB}(t,x,y,x_0)dx_0. \tag{6.6}$$

The technique for estimating the initial error can be carried out in multi-dimensional setting, without any further difficulty.

As for the evolution error, some clarification of the notation needs to be done. For example, the main representations (5.1)-(5.6), can be reformulated as follows:

$$I_{jn} = \frac{\varepsilon^{j-\frac{d}{2}}}{(2\pi)^{\frac{d}{2}}}\int_{K_0}\sum_{|\beta|=(3-2j)_+} G_{jn\beta}(t,x,y;x_0)(x-\tilde{x}_n(t;x_0))^\beta e^{i\Phi_n(t,x;x_0)/\varepsilon}dx_0, \tag{6.7}$$

where

$$G_{0n\beta}(t,x;x_0,y) = \frac{1}{\beta!}a_n(t;x_0)\partial_x^\beta F_n(t,x^*)z_n(k,y), \quad |\beta| = 3, \tag{6.8}$$

$$G_{1n\beta}(t,x;x_0) = (ia\langle\partial_k z_n, z_n\rangle\dot{M}_n(t;x_0) - \sum_{|\beta|=3}\frac{1}{\beta!}\partial_x^\beta F_n(t,x^*)A_{1n}(x-\tilde{x})^{(\beta-1)_+}), \tag{6.9}$$

$$G_{2n}(t,x;x_0,y) = a_n(t;x_0)(Tr(M_n))^2\Delta_k z_n(k_n,y) + iLA_{1n}. \tag{6.10}$$

Finally,

$$J_{jn}(x,y,x_0,x_0') = \frac{\varepsilon^{2j-d}}{(2\pi)^d}\sum_{|\beta|=(3-2j)_+}(G_{jn\beta}(t,x,y;x_0))(x-\tilde{x}_n(t;x_0))^\beta \times \sum_{|\beta|=(3-2j)_+}\overline{(G_{jn\beta}(t,x,y;x_0'))}(x-\tilde{x}_n(t;x_0'))^\beta e^{i\psi_n/\varepsilon}.$$

The rest of the ingredients of the proof remain unchanged, except when using the non-stationary phase method K needs to be taken as $d+1$.

Another possible extension of this result is to apply our technique to higher order Gaussian beam superpositions, using the Gaussian beam construction in [**14**].

Our results valid for a finite number of bands can be used in practice by approximating a given high frequency initial data by a finite number of bands within

certain accuracy. An open question is to deal with infinite number of bands, which is left to a future work.

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On random weighted Sobolev inequalities on $\mathbb{R}^d$ and applications

Didier Robert and Laurent Thomann

Abstract. Our aim in this paper is to give an overview of recent results concerning randomization methods applied to Schrödinger equations obtained in previous work by the authors. We focus here on properties of the harmonic oscillator and Hermite functions for simplicity.

The general idea is that several well known deterministic results like Sobolev type inequalities are improved in a large extent by introducing some randomness. This is very useful in particular for N.L.S with supercritical initial data.

1. Introduction

We present here the results we have obtained in [**32**, **33**] in collaboration with Aurélien Poiret and the results of [**35**]. Using ideas of Shiffman-Zelditch [**37**] and Burq-Lebeau [**6**] who developed a randomisation method based on the Laplace operator on a compact Riemannian manifold, we give a randomisation method on $L^2(\mathbb{R}^d)$ associated with the Laplace operator with confining potentials. We are able to construct probability measures on $L^2(\mathbb{R}^d)$, on the support of which a typical function enjoys better Sobolev estimates than expected. These measures and estimates have an interest in themselves, but we can moreover use them to

- construct orthonormal bases of $L^2(\mathbb{R}^d)$ of Hermite functions which enjoy good L^∞ bounds. These bounds are shown to be optimal ;
- prove quantum ergodicity results ;
- show a.s. local and global well-posedness results for supercritical nonlinear Schrödinger equations with quadratic potential ;
- show a.s. global well-posedness results for supercritical nonlinear Schrödinger equations (without potential).

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To simplify the exposition, we will focus on estimates in the Sobolev spaces based on the harmonic oscillator in $L^2(\mathbb{R}^d)$

$$H = -\Delta + |x|^2 = \sum_{j=1}^{d} (-\partial_j^2 + x_j^2).$$

We get optimal stochastic weighted Sobolev estimates on $\mathbb{R}^d$ using the Burq-Lebeau method. In [**6**], the construction of the measures relied on Gaussian random variables but it is possible to consider general random variable which satisfy concentration of measure estimates (like Bernoulli random variables). However, the optimal estimates (including lower bounds) are obtained only for the Gaussian law.

Let us emphasise here that even if there exist many similarities between the spectral properties of the Laplace operators a compact Riemannian manifolds and Schrödinger Hamiltonians with a confining potential on $\mathbb{R}^d$, there exists a big difference due to the complex behaviour at high energy of the spectral function on a non-compact configuration space.

In [**35**] we prove that most of the results can be extended to more general Schrödinger Hamiltonians $-\triangle + V(x)$ with confining potentials V.

2. Spectral estimates and harmonic Sobolev spaces

Let us recall the well known spectral analysis of the quantum harmonic oscillator H on $\mathbb{R}^d$. This is explained in many text books on quantum mechanics. For mathematical details, we refer to Helffer [**20**] or to the course of Ramond [**34**].

The operator H is self-adjoint on the Hilbert space $L^2(\mathbb{R}^d)$, and has the discrete spectrum $\{2n+d\}_{n\in\mathbb{N}}$.

- For $d = 1$ each eigenvalue is simple, $H\mathfrak{h}_n = (2n+d)\mathfrak{h}_n$ where $\mathfrak{h}_n$ is the n^{th} Hermite function.
- For $d \geq 2$, an orthonormal basis is obtained by tensor products. Let $\alpha = (\alpha_1, \cdots, \alpha_d) \in \mathbb{N}^d$, $x = (x_1, \cdots, x_d) \in \mathbb{R}^d$,

$$\mathfrak{h}_\alpha(x) = \mathfrak{h}_{\alpha_1}(x_1) \cdots \mathfrak{h}_{\alpha_d}(x_1), \quad \alpha_1 + \cdots + \alpha_d = n. \tag{2.1}$$

It is sometimes convenient to use different notations. Any orthonormal basis of $\ker(H-(2n+d))$ can be denoted by $\{\varphi_{n,k}\}_{1\leq k\leq m_n}$, so that $H\varphi_{n,k} = (2n+d)\varphi_{n,k}$. In the sequel, $\{\lambda_j\}_{j\in\mathbb{N}}$ denotes the non-decreasing sequence of eigenvalues where each eigenvalue $(2n+d)$ is repeated according its multiplicity, such that $H\varphi_j = \lambda_j\varphi_j$ where $\{\varphi_j\}_{j\geq 0}$ is an orthonormal basis of $L^2(\mathbb{R}^d)$.

By (2.1) the multiplicity of the eigenvalue $2n+d$ is of order n^{d-1}, therefore λ_j is of order $j^{1/d}$.

The scale of harmonic Sobolev spaces is defined as follows: $s \geq 0$, $p \geq 1$.

$$\mathcal{W}^{s,p} = \mathcal{W}^{s,p}(\mathbb{R}^d) = \left\{u \in L^p(\mathbb{R}^d),\ H^{s/2}u \in L^p(\mathbb{R}^d)\right\}, \tag{2.2}$$

$$\mathcal{H}^s = \mathcal{H}^s(\mathbb{R}^d) = \mathcal{W}^{s,2}.$$

The natural norms are denoted by $\|u\|_{\mathcal{W}^{s,p}}$ and up to equivalence of norms we have (see [**41**, Lemma 2.4]) for $1 < p < +\infty$

$$\|u\|_{\mathcal{W}^{s,p}} = \|H^{s/2}u\|_{L^p} \equiv \|(-\Delta)^{s/2}u\|_{L^p} + \|\langle x\rangle^s u\|_{L^p}.$$

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For $s \geq 0$, $\mathcal{H}^s$ is the domain of the self-adjoint operator $H^{s/2}$ and we have

$$\mathcal{H}^s = \big\{ u \in L^2(\mathbb{R}^d),\ \sum_{j\geq 0} \lambda_j^s |\langle \varphi_j, u\rangle|^2 < +\infty \big\}$$

and

$$\|u\|^2_{\mathcal{H}^s} \approx \sum_{j\geq 0} \lambda_j^s |\langle \varphi_j, u\rangle|^2.$$

In the sequel we fix $d \geq 2$. Let us consider spectral windows I_h depending on a small parameter $h > 0$ (this notation is convenient to make use of semiclassical results here and in the more general setting considered in [**35**]).

Let us denote by $I_h = [\frac{a_h}{h}, \frac{b_h}{h}[$ and assume that a_h and b_h satisfy, for some a, b, $D > 0$ and $\delta \in [0, 1]$,

$$\lim_{h\to 0} a_h = a, \quad \lim_{h\to 0} b_h = b, \quad 0 < a \leq b \quad \text{and} \quad b_h - a_h \geq D h^\delta, \tag{2.3}$$

with any $D > 0$ if $\delta < 1$ and $D \geq 2$ in the case $\delta = 1$. This condition ensures that N_h, the number (with multiplicities) of eigenvalues of H in I_h tends to infinity when $h \to 0$. Indeed, we can check that $N_h \sim c h^{-d}(b_h - a_h)$, in particular $\lim_{h\to 0} N_h = +\infty$, since $d \geq 2$. In the sequel, we write $\Lambda_h = \{j \geq 1,\ \lambda_j \in I_h\}$ and $\mathcal{E}_h = \operatorname{span}\{\varphi_j,\ j \in \Lambda_h\}$, so that $N_h = \#\Lambda_h = \dim \mathcal{E}_h$. Finally, we denote by $\mathbf{S}_h = \big\{u \in \mathcal{E}_h\ :\ \|u\| = 1\big\}$ the unit sphere of $\mathcal{E}_h$ (which is a complex linear space of dimension N_h).

A very useful tool to get local and global estimates in the deterministic setting as well as in the probabilistic setting are L^p estimates of spectral projectors and of their kernels, the so-called spectral function. On compact manifolds this is obvious in [**38**] for example.

The spectral function is then defined as

$$\pi_H(\lambda; x, y) = \sum_{\lambda_j \leq \lambda} \varphi_j(x)\overline{\varphi_j(y)}$$

(recall that this definition does not depend on the choice of $\{\varphi_j, j \in \mathbb{N}\}$). When the energy λ is localized in $I \subseteq \mathbb{R}^+$ we denote by $\Pi_H(I)$ the spectral projector of H on I. The range $\mathcal{E}_H(I)$ of $\Pi_H(I)$ is spanned by $\{\varphi_j; \lambda_j \in I\}$ and $\Pi_H(I)$ has an integral kernel given by

$$\pi_H(I; x, y) = \sum_{[j\,:\,\lambda_j \in I]} \varphi_j(x)\overline{\varphi_j(y)}.$$

We will also use the notation $\mathcal{E}_H(\lambda) = \mathcal{E}_H([0, \lambda])$, $N_H(\lambda) = \dim[\mathcal{E}_H(\lambda)]$.

The relationship between Sobolev type estimates and the spectral function is illustrated by the following elementary result:

$$|u(x)| \leq (\pi_H(I; x, x))^{1/2} \|u\|_{L^2(\mathbb{R}^d)}. \tag{2.4}$$

We have the following uniform estimate:

$$\pi_H(\lambda; x, x) \leq C_\theta \lambda^{(d+\theta)/2} \langle x\rangle^{-\theta},$$

where C_θ depends only on $\theta > 0$. Now using (2.4) we get (with the semiclassical parameter $h = \lambda^{-1}$)

$$\langle x\rangle^{\theta/2} h^{(d+\theta)/4} |u(x)| \leq C_\theta \|u\|_{L^2(\mathbb{R}^d)}, \quad \forall u \in \mathcal{E}_H(h^{-1}).$$

For smaller spectral windows like I_h we need more accurate estimates on the spectral function

$$e_x := \pi_H(\frac{b_h}{h}; x, x) - \pi_H(\frac{a_h}{h}; x, x).$$

For any $\theta \geq 0$ there exists $C_\theta > 0$ such that

$$\langle x\rangle^\theta e_x \leq C_\theta N_h h^{(d-\theta)/2}. \tag{2.5}$$

where C_θ depends only on $\theta \geq 0$. Using (2.4) and interpolation inequalities we get Sobolev type inequalities for $u \in \mathcal{E}_h$, $\theta \geq 0$, $p \geq 2$

$$\|u\|_{L^{\infty,\theta/2}(\mathbb{R}^d)} \leq C\left(N_h h^{(d-\theta)/2}\right)^{1/2} \|u\|_{L^2(\mathbb{R}^d)}, \tag{2.6}$$

which in turn implies using interpolation

$$\|u\|_{L^{p,\theta(p/2-1)}(\mathbb{R}^d)} \leq C\left(N_h h^{(d-\theta)/2}\right)^{\frac{1}{2}-\frac{1}{p}} \|u\|_{L^2(\mathbb{R}^d)}. \tag{2.7}$$

The previous inequality can be written as

$$\|u\|_{L^{p,\theta(p/2-1)}(\mathbb{R}^d)} \leq C(b_h - a_h)^{\frac{1}{2}-\frac{1}{p}} h^{-(\frac{d+\theta}{2})(\frac{1}{2}-\frac{1}{p})} \|u\|_{L^2(\mathbb{R}^d)},$$
$$\forall p \in [2, +\infty],\ \forall \theta \in [0, d].$$

We shall see that these Sobolev type inequalities in a large extent can be improved in a random sense that we shall explain now.

3. Probabilistic weighted estimates for frequency localized functions

3.1. Probabilistic setting. Let us introduce now our probabilistic setting. Consider a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and let $\{X_n,\ n \geq 1\}$ be a sequence of i.i.d random variables, centered and normalized following a law ν. We assume for simplicity in all this paper that ν **is either the standard complex Gaussian** $\mathcal{N}_{\mathbb{C}}(0,1)$ **or the Bernoulli law** $\frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_1$ (see [**33**] for more general laws satisfying a concentration of measure property).

Let $\gamma := (\gamma_n)_{n\in\mathbb{N}}$ be a sequence of complex numbers and define the random vector in $\mathcal{E}_h$

$$v_\gamma(\omega) := \sum_{j\in\Lambda_h} \gamma_j X_j(\omega)\varphi_j. \tag{3.1}$$

The probability law of v_γ is denoted by ν_γ. We define a probability measure $\mathbf{P}_\gamma$ on the sphere $\mathbf{S}_h$ by: for all measurable and bounded function $f : \mathbf{S}_h \longrightarrow \mathbb{R}$,

$$\int_{\mathbf{S}_h} f(u)\mathrm{d}\mathbf{P}_\gamma(u) = \int_\Omega f\Big(\frac{v_\gamma(\omega)}{\|v_\gamma(\omega)\|_{L^2(\mathbb{R}^d)}}\Big)\mathrm{d}\mathbb{P}(\omega).$$

It is not difficult to see that in the isotropic case ($\gamma_j = \frac{1}{\sqrt{N_h}}$ for all $j \in \Lambda_h$) and when $X_j \sim \mathcal{N}_{\mathbb{C}}(0,1)$, then $\mathbf{P}_\gamma$ is the uniform probability on the sphere $\mathbf{S}_h$.

For more general sequences γ we need to assume the following squeezing conditions. There exists $K_0 > 0$, $K_1 > 0$ such that

$$\|\gamma\|_{\ell^\infty(\Lambda_h)} \leq \frac{K_0}{\sqrt{N_h}}\|\gamma\|_{\ell^2(\Lambda_h)}, \quad \forall h \in]0, 1]. \tag{3.2}$$

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We also need the stronger condition

$$\frac{K_1}{\sqrt{N_h}}\|\gamma\|_{\ell^2(\Lambda_h)} \leq |\gamma_j| \leq \frac{K_0}{\sqrt{N_h}}\|\gamma\|_{\ell^2(\Lambda_h)}, \quad \forall h \in]0,1],\ \forall j \in \Lambda_h. \tag{3.3}$$

Notice that

$$\mathbb{E}(\|v_\gamma\|^2_{L^2(\mathbb{R}^d)}) = \sum_{j\in\Lambda_h} |\gamma_j|^2 = |\gamma|^2_{\ell^2(\Lambda_h)}.$$

Let us comment now our assumptions.

REMARK 3.1. *(i) Assumptions (3.2) and (3.3) mean that in the index set Λ_h the sequence γ is almost constant. In applications it is useful to be able to modify the γ_j. By considering two sequences γ, β and using the Kakutani theorem we can construct mutually singular probability measures μ_γ, μ_β on the Sobolev space $\mathcal{H}^s$ (see* [**33**, Section 2.2]*). In particular this gives larger sets of initial data for solutions of NLS (see Section* 6.2 *of this paper).*

(ii) Assumptions (3.2) and (3.3) are very useful to be able to use the accurate spectral estimate (2.5) as we have shown in [**33**, Section 3]*. This condition allows to normalize the $\mathcal{H}^s$-norm of v_γ. Moreover it is compatible with the Lévy contraction principle (see* [**22**] *for details).*

(iii) It is possible to avoid assumption (3.2) at the price of introducing new weighted Sobolev spaces (see the definition of the space $\mathcal{Z}$ in [**22**]*).*

(iv) The Gaussian complex law is natural because it gives the uniform probability measure on the sphere $\mathbf{S}_h$, but in this case the $\mathcal{H}^s$-norm of v_γ (3.1) depends on ω. This is not the case if ν is a centred Bernoulli law. Moreover the probabilistic information we get clearly depends on ν and it may be interesting to consider also discrete probability laws. Actually, our results are proven under the assumption that the family $(\nu^{\otimes N}, \mathbb{R}^N)_{N\geq 1}$ satisfies the concentration property of measures. Finally, we point out that the results of Section 6 *hold true under the weaker assumption that ν is sub-gaussian: there exists $\sigma \geq 0$ such that*

$$\int_{\mathbb{R}} \mathrm{e}^{sx} d\nu(x) \leq \mathrm{e}^{\frac{\sigma^2}{2}s^2}, \ \ \forall s \in \mathbb{R}.$$

For a discussion about these conditions we refer to [**33**, Section 2.1].

A very useful tool here is a measure concentration property satisfied by the probability $\mathbf{P}_\gamma$, proved by P. Lévy for the uniform law. For a study of this notion, we refer to the book [**25**].

PROPOSITION 3.1. *Suppose that Assumption* (3.3) *is satisfied. Then there exist constants $K > 0$, $\kappa > 0$ such that for every Lipschitz function $F : \mathbf{S}_h \longrightarrow \mathbb{R}$ satisfying*

$$|F(u) - F(v)| \leq \|F\|_{Lip}\|u - v\|_{L^2(\mathbb{R}^d)}, \quad \forall u, v \in \mathbf{S}_h,$$

we have

$$\mathbf{P}_\gamma\Big[\, u \in \mathbf{S}_h : |F - \mathcal{M}_F| > r \,\Big] \leq K\mathrm{e}^{-\frac{\kappa N_h r^2}{\|F\|^2_{Lip}}}, \quad \forall r > 0, \ \ h \in]0,1], \tag{3.4}$$

where $\mathcal{M}_F$ is a median for F.

Recall that a median $\mathcal{M}_F$ for F is defined by

$$\mathbf{P}_\gamma\big[\, u \in \mathbf{S}_h : F \geq \mathcal{M}_F \,\big] \geq \frac{1}{2}, \quad \mathbf{P}_\gamma\big[\, u \in \mathbf{S}_h : F \leq \mathcal{M}_F \,\big] \geq \frac{1}{2}.$$

The factor N_h in the exponential of r.h.s of (3.4) is crucial in applications to get large deviation estimates.

3.2. L^p bounds, $2 \leq p < +\infty$. The following result shows that for $\theta = d$ the Sobolev estimate (2.7) is improved by the factor $N_h^{\frac{1}{p}-\frac{1}{2}}$ for u in a set of probability close to 1.

THEOREM 3.1 ([**33**], Theorem 4.7). *Let $p \geq 2$. Denote by $\mathcal{M}_p$ a median of $\|u\|_{L^{p,d(p/2-1)}}$. Assume condition (3.2) and let $\delta \in [0,1]$. Then there exist $0 < C_0 < C_1$, $K > 0$, $c_1 > 0$, $h_0 > 0$ such that for all $r \in [2, K|\log h|]$ and $h \in]0, h_0]$ such that*

$$\mathbf{P}_{\gamma,h}\Big[u \in \mathbf{S}_h : \Big|\|u\|_{L^{p,d(p/2-1)}} - \mathcal{M}_p\Big| > \Lambda\Big] \leq 2\exp\big(-c_2 N_h^{2/p}\Lambda^2\big). \tag{3.5}$$

Moreover if condition (3.3) is satisfied and if $\delta \in [0, 2/3[$, then we have

$$C_0\sqrt{p} \leq \mathcal{M}_p \leq C_1\sqrt{p}, \quad \forall p \in [2, K\log N_h].$$

This result shows that $\|u\|_{L^{p,d(p/2-1)}}$ has a Gaussian concentration around its median. The first part of the theorem is a direct application of Proposition 3.1 to $F(u) = \|u\|_{L^{p,d(p/2-1)}}$. The estimate of $\mathcal{M}_p$ is more involved and needs the following estimate for the spectral function.

LEMMA 3.1 ([**33**], Lemma 4.9). *Let $\delta \in [0, 2/3[$ and $-d/(p-1) < \theta \leq 1$. There exist $0 < C_0 < C_1$ and $h_0 > 0$ such that*

$$C_0 N_h h^{\frac{d-\theta}{2}(1-\frac{1}{p})} \leq \left(\int_{\mathbb{R}^d} \langle x\rangle^{\theta(p-1)} e_x^p \, dx\right)^{1/p} \leq C_1 N_h h^{\frac{d-\theta}{2}(1-\frac{1}{p})},$$

for every $p \in [1, \infty[$ and $h \in]0, h_0]$.

Let $0 < \eta < 1$, then we are able to precise the concentration estimate (3.5) in the regime $p \sim |\ln h|^{1-\eta}$. Assume that for all $j \in \Lambda_h$, $\gamma_j = N_h^{-1/2}$ and that $X_j \sim \mathcal{N}_{\mathbb{C}}(0,1)$, so that $\mathbf{P} := \mathbf{P}_\gamma$ is the uniform probability on $\mathbf{S}_h$.

THEOREM 3.2. *Let $\delta \in [0, 2/3[$, $0 < \eta < 1$ and set $p_h = |\ln h|^{1-\eta}$. Then there exists constants $C_\star = C_\star(d)$ and $c > 0$ such that for all $\varepsilon > 0$ there exists $h_0 > 0$ so that for all $h \in]0, h_0]$*

$$\mathbf{P}_{\gamma,h}\Big[u \in \mathbf{S}_h : \Big|\|u\|_{L^{p_h,d(p_h/2-1)}} - C_\star\sqrt{p_h}\Big| > \varepsilon\sqrt{p_h}\Big] \leq 2e^{-c\varepsilon^2|\ln h|}.$$

We give the main lines of the proof in the appendix.

3.3. L^∞ bounds. The next result shows that for $\theta = d$ the Sobolev estimate (2.6) is improved by the factor $N_h^{-\frac{1}{2}}|\log h|$ for u in a set of probability close to 1. We suppose that (3.2) and (2.3) with $0 \leq \delta \leq 1$ are satisfied.

THEOREM 3.3 ([**33**], Theorem 4.1). *There exist $h_0 \in]0,1]$, $c_2 > 0$ and $C > 0$ such that if $c_1 = d(1 + d/4)$, we have*

$$\mathbf{P}_{\gamma,h}\Big[u \in \mathbf{S}_h : \ h^{-\frac{d-\theta}{4}}\|u\|_{L^{\infty,\theta/2}(\mathbb{R}^d)} > \Lambda\Big] \leq Ch^{-c_1}\mathrm{e}^{-c_2\Lambda^2}, \ \forall \Lambda > 0, \ \forall h \in]0, h_0].$$

We can deduce probabilistic estimates for the derivatives as well. Recall that the Sobolev spaces $\mathcal{W}^{s,p}(\mathbb{R}^d)$ are defined in (2.2). The following result say that Theorem 3.3 is sharp for large enough spectral windows.

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THEOREM 3.4 ([**33**], Theorem 1.1). *Let $d \geq 2$. Assume that $0 \leq \delta < 2/3$ in (2.3) and that condition (3.3) holds. Then there exist $0 < C_0 < C_1$, $c_1 > 0$ and $h_0 > 0$ such that for all $h \in]0, h_0]$.*

$$\mathbf{P}_{\gamma,h}\left[u \in \mathbf{S}_h : C_0|\log h|^{1/2} \leq \|u\|_{\mathcal{W}^{d/2,\infty}(\mathbb{R}^d)} \leq C_1|\log h|^{1/2}\right] \geq 1 - h^{c_1}.$$

It is clear that under condition (3.3), there exist $0 < C_2 < C_3$, so that for all $u \in \mathbf{S}_h$, and $s \geq 0$

$$C_2 h^{-s/2} \leq \|u\|_{\mathcal{H}^s(\mathbb{R}^d)} \leq C_3 h^{-s/2},$$

since all elements of $\mathbf{S}_h$ oscillate with frequency $h^{-1/2}$. Thus Theorem 3.4 shows a gain of $d/2$ derivatives in L^∞, and this induces a gain of d derivatives compared to the usual deterministic Sobolev embeddings. This can be compared with the results of [**6**] where the authors obtain a gain of $d/2$ derivatives on compact manifolds: this comes from different behaviours of the spectral function, see Section 2. Notice that the bounds in Theorem 3.4 (and in the results of [**6**] as well) do not depend on the length of the interval of the frequency localisation I_h (see (2.3)), but only on the size of the frequencies. This is a consequence of the randomisation, and from the bound (2.5).

In our works we give estimates for the eigenfunctions in the configuration space, while Feng, Shiffman and Zelditch [**19**, **37**] give similar estimates in the Bargmann representation for holomorphic fields.

We now state a result which gives optimal L^∞ bounds in the general case $0 \leq \delta \leq 1$

THEOREM 3.5. *Let $d \geq 2$. Assume that $0 \leq \delta \leq 1$ in (2.3) and that condition (3.3) holds. Then there exist $0 < C_0 < C_1$, $c_1 > 0$ and $h_0 > 0$ such that for all $h \in]0, h_0]$.*

$$\mathbf{P}_{\gamma,h}\left[u \in \mathbf{S}_h : C_0|\log h|^{1/2} \leq h^{-d/4}\|u\|_{L^\infty(\mathbb{R}^d)} \leq C_1|\log h|^{1/2}\right] \geq 1 - h^{c_1}.$$

We will give the main lines of the proof of this result in the Appendix B. The key obervation is that the estimates of the L^p norm of the spectral function (which are not optimal when δ is close to 1), become optimal in the regime $p = p_h \sim c|\ln h|$.

4. Hermite functions estimates

In this section the previous results are applied to obtain L^∞ estimates for Hermite functions.

THEOREM 4.1 ([**33**], Theorem 1.3). *Let $d \geq 2$. Then there exists an orthonormal basis of $L^2(\mathbb{R}^d)$ of eigenfunctions of the harmonic oscillator H denoted by $\{\varphi_n^\sharp\}_{n\geq 1}$ such that $\|\varphi_n^\sharp\|_{L^2(\mathbb{R}^d)} = 1$ and so that for some $M > 0$ and all $n \geq 1$,*

$$\|\varphi_n^\sharp\|_{L^\infty(\mathbb{R}^d)} \leq M\lambda_n^{-\frac{d}{4}}(1 + \log\lambda_n)^{1/2}. \tag{4.1}$$

In other words, all elements of this basis are decreasing in $L^\infty(\mathbb{R}^d)$ norm.

Let us compare (4.1) with the general known bounds on Hermite functions. We have $H\varphi_n = \lambda_n\varphi_n$, with $\lambda_n \sim cn^{1/d}$, therefore (4.1) can be rewritten

$$\|\varphi_n^\sharp\|_{L^\infty(\mathbb{R}^d)} \leq Mn^{-1/4}(1 + \log n)^{1/2},\ \forall n \geq 0., \tag{4.2}$$

For a general orthonormal basis of Hermite functions, with $d \geq 2$, Koch and Tataru [**23**] (see also [**24**]) prove that

$$\|\varphi_n\|_{L^\infty(\mathbb{R}^d)} \leq C\lambda_n^{\frac{d}{4}-\frac{1}{2}},$$

which shows that (4.2) induces a gain of $d-1$ derivatives compared to the general case.

Notice that for the tensorial Hermite basis $\mathfrak{h}_\alpha(x)$, using the bound for $d=1$ [**23**, **40**] we have

$$\|\mathfrak{h}_\alpha\|_{L^\infty(\mathbb{R}^d)} \leq C\lambda_n^{-\frac{1}{12}}, \quad \text{for } \alpha_1+\cdots+\alpha_d=\lambda_n.$$

Observe also that the basis of radial Hermite functions does not satisfy (4.1) in dimension $d \geq 2$, as we have recently proved in [**22**]. We will see in Theorem 4.3 that the log term in (4.1) can not be avoided.

Theorem 4.1 is a consequence of a more powerful result, obtained following an idea in [**43**]. Here we follow the main lines of [**6**, Section 3]. In this part the upper bounds estimates of Section 3 are used in their full strength.

Firstly, we assume that for all $j \in \Lambda_h$, $\gamma_j = N_h^{-1/2}$ and that $X_j \sim \mathcal{N}_{\mathbb{C}}(0,1)$, so that $\mathbf{P} := \mathbf{P}_\gamma$ is the uniform probability on $\mathbf{S}_h$. We set $h_k = 1/k$ with $k \in \mathbb{N}^*$, and

$$a_{h_k} = 2 + dh_k, \quad b_{h_k} = 2 + (2+d)h_k.$$

Then (2.3) is satisfied with $\delta = 1$ and $D = 2$. In particular, each interval

$$I_{h_k} = \Big[\frac{a_{h_k}}{h_k}, \frac{b_{h_k}}{h_k}\Big[= [2k+d, 2k+d+2[$$

only contains the eigenvalue $2k+d$ with multiplicity $N_{h_k} \sim ck^{d-1}$, and $\mathcal{E}_{h_k}$ is the corresponding eigenspace of the harmonic oscillator H. We can identify the space of the orthonormal basis of $\mathcal{E}_{h_k}$ with the unitary group $U(N_{h_k})$ and we endow $U(N_{h_k})$ with its Haar probability measure ρ_k. Then the space $\mathcal{B}$ of the Hilbertian bases of eigenfunctions of H in $L^2(\mathbb{R}^d)$ can be identified with

$$\mathcal{B} = \times_{k\in\mathbb{N}} U(N_{h_k}), \tag{4.3}$$

which can be endowed with the measure

$$\mathrm{d}\rho = \otimes_{k\in\mathbb{N}} \mathrm{d}\rho_k. \tag{4.4}$$

Denote by $B = (\varphi_{k,\ell})_{k\in\mathbb{N},\, \ell\in[\![1,N_{h_k}]\!]} \in \mathcal{B}$ a typical orthonormal basis of $L^2(\mathbb{R}^d)$ so that for all $k \in \mathbb{N}$, $(\varphi_{k,\ell})_{\ell\in[\![1,N_{h_k}]\!]} \in U(N_{h_k})$ is an orthonormal basis of $\mathcal{E}_{h_k}$.

Then the main result of the section which implies Theorem 4.1, is the following.

THEOREM 4.2 ([**33**], Theorem 5.1). *Let $d \geq 2$. Then, if $M > 0$ is large enough, there exist $c, C > 0$ so that for all $r > 0$*

$$\rho\Big[B = (\varphi_{k,\ell})_{k\in\mathbb{N},\, \ell\in[\![1,N_{h_k}]\!]} \in \mathcal{B} : \exists k,\ell; \\ \|\varphi_{k,\ell}\|_{\mathcal{W}^{d/2,\infty}(\mathbb{R}^d)} \geq M(\log k)^{1/2} + r \Big] \leq C\mathrm{e}^{-cr^2}.$$

The previous result relies on the following proposition

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PROPOSITION 4.1 ([**33**], Proposition 5.2). *Let $d \geq 2$. Then, if $M > 0$ is large enough, there exist $c, C > 0$ so that for all $r > 0$ and $k \geq 1$*

$$\rho_k\Big[B_k = (\psi_\ell)_{\ell \in [\![1, N_{h_k}]\!]} \in U(N_{h_k}) : \exists \ell \in [\![1, N_{h_k}]\!]; \\ \|\psi_\ell\|_{\mathcal{W}^{d/2,\infty}(\mathbb{R}^d)} \geq M(\log k)^{1/2} + r \Big] \leq Ck^{-2}\mathrm{e}^{-cr^2}.$$

Let us show how this result implies Theorem 4.2: We set

$$\mathcal{F}_{k,r} = \big\{ B_k = (\psi_\ell)_{\ell \in [\![1, N_{h_k}]\!]} \in U(N_{h_k}) : \forall \ell \in [\![1, N_{h_k}]\!]; \\ \|\psi_\ell\|_{\mathcal{W}^{d/2,\infty}(\mathbb{R}^d)} \leq M(\log k)^{1/2} + r \big\},$$

and $\mathcal{F}_r = \cap_{k \geq 1} \mathcal{F}_{k,r}$. Then for all $r > 0$

$$\rho(\mathcal{F}_r^c) \leq \sum_{k \geq 1} \rho_k(\mathcal{F}_{k,r}^c) \leq C \sum_{k \geq 1} k^{-2}\mathrm{e}^{-cr^2} = C'\mathrm{e}^{-cr^2},$$

and this completes the proof.

Then from the Borel-Cantelli Lemma we get

COROLLARY 4.1 ([**33**], Corolllary 5.3). *For ρ-almost all orthonormal basis $(\varphi_{k,\ell})_{k \in \mathbb{N},\, \ell \in [\![1, N_{h_k}]\!]}$ of eigenfunctions of H we have*

(i) For $2 \leq p < +\infty$

$$\|\varphi_{k,\ell}\|_{L^p(\mathbb{R}^d)} \leq C_p k^{-\frac{d}{2}(\frac{1}{2} - \frac{1}{p})}, \qquad \forall\, k \in \mathbb{N},\ \forall\, \ell \in [\![1, N_{h_k}]\!].$$

(ii) For $p = +\infty$

$$\|\varphi_{k,\ell}\|_{L^\infty(\mathbb{R}^d)} \leq (M+1)k^{-d/4}(1 + \log k)^{1/2}, \qquad \forall\, k \in \mathbb{N},\ \forall\, \ell \in [\![1, N_{h_k}]\!].$$

We now state a result we shows that the log factor in the previous bounds is optimal

THEOREM 4.3. *Let $d \geq 2$. Then for all $M > 0$*

$$\rho\Big[B = (\varphi_{k,\ell})_{k \in \mathbb{N},\, \ell \in [\![1, N_{h_k}]\!]} \in \mathcal{B} :\ \liminf_{k \to +\infty} \inf_{\ell = 1, \ldots, N_k} k^{d/4} \|\varphi_{k,\ell}\|_{L^\infty(\mathbb{R}^d)} \leq M \Big] = 0.$$

This means that, from an orthonormal basis, one cannot extract a subsequence which satisfies better bounds than in Corollary 4.1.

This result is a consequence of Theorem 3.5. For the proof, we can follow the main lines of [**6**, Théorème 8] where an analogous result for the spherical harmonics is proven.

5. Application to quantum ergodicity

Recall that "quantum ergodicity" for a quantum Hamiltonian H usually means that in some semiclassical regime almost all eigenfunctions of H are distributed according to an invariant measure with a support equal to the classical energy shell.

Assume that $I_h =]a_h, b_h]$ is such that

$$\lim_{h \to 0} a_h = \lim_{h \to 0} b_h = \eta > 0 \qquad \text{and} \qquad \lim_{h \to 0} \frac{b_h - a_h}{h} = +\infty.$$

The Liouville measure L_η associated with the classical Hamiltonian $H_{c\ell}(x,\xi) = |x|^2 + |\xi|^2$ is here the uniform probability on the sphere $\sqrt{\eta}\,\mathbb{S}^{2d-1}$. We define the class of symbols

$$S(1) = \big\{ A \in C^\infty(\mathbb{R}^{2d}),\ \forall \alpha, \forall \beta,\ \sup_{(x,\xi)} |\partial_x^\alpha \partial_\xi^\beta A(x,\xi)| < +\infty \big\},$$

and $S(1,1) \subset S(1)$ the class of symbols such that $A \in C^\infty(\mathbb{R}^{2d})$ and A is homogeneous of degree 0 outside a small neighbourhood of $(0,0)$ in $\mathbb{R}^d_x \times \mathbb{R}^d_\xi$: $A(\lambda x, \lambda\xi) = A(x,\xi)$ for every $\lambda \geq 1$ and $|(x,\xi)| \geq \varepsilon$.

For $A \in S(1)$ let us denote by $\hat{A}$ the Weyl quantization of A (here $h = 1$). Notice that if $\|u_h\|_{L^2(\mathbb{R}^d)} = 1$ then $A \mapsto \langle u_h, \hat{A} u_h\rangle$ defines a semiclassical measure on $\sqrt{\eta}\,\mathbb{S}^{2d-1}$ (see e.g. [**5**]).

Then we have

THEOREM 5.1 ([**35**], Theorem 1.4). *Assume that we are in the isotropic case ($\gamma_j = \frac{1}{\sqrt{N_h}}$ for all $j \in \Lambda_h$). Then there exist $c, C > 0$ so that for all $r \geq 1$ and $A \in S(1,1)$,*

$$\mathbf{P}_h\Big[u \in \mathbf{S}_h : |\langle u, \hat{A} u\rangle - L_\eta(A)| > r \Big] \leq C e^{-cN_h r^2},\ \ \forall h \in]0,1]. \tag{5.1}$$

This result can be related with quantum ergodicity (see [**15**, **21**, **26**, **42**] and the book [**46**, Chapter 15] for an introduction to this subject) which concerns the semiclassical behavior of $\langle \varphi_j, \hat{A}\varphi_j\rangle$ when the classical flow is ergodic on the energy hyper surface $H_{c\ell}^{-1}(\eta)$. Then, for "almost all" eigenfunctions φ_j, we have $\langle \varphi_j, \hat{A}\varphi_j\rangle \overset{j\to+\infty}{\longrightarrow} L_\eta(A)$. The meaning of Theorem 5.1 is that we have $\langle u, \hat{A} u\rangle \overset{h\to 0}{\longrightarrow} L_\eta(A)$ for almost all $u \in \mathbf{S}_h$ such that all modes $(\varphi_j)_{j\in\Lambda_h}$ are "almost uniformly distributed" in u. For related results on compact manifolds see Zelditch [**44**].

As a consequence of Theorem 5.1 we get easily that almost all bases of Hermite functions is Quantum Uniquely Ergodic (see Theorem 5.2 for a precise statement). In [**43**] the author proved that on the standard sphere a random orthonormal basis of eigenfunctions of the Laplace operator is ergodic.

Burq-Lebeau [**6**, Théorème 3] obtained a similar result for the Laplacian on a compact manifold. A modification of their proof allows to consider more general random variables satisfying the Gaussian concentration assumption instead of the uniform law.

From (5.1) we directly deduce that there exists $C > 0$ so that for all $p \geq 2$ and $h \in]0,1]$,

$$\big\| \langle u, \hat{A} u\rangle - L_\eta(A) \big\|_{L^p_{\mathbf{P}_h}} \leq C N_h^{-1/2} \sqrt{p}.$$

Therefore, if one denotes by

$$u_h^\omega = \frac{1}{\sqrt{N_h}} \sum_{j\in\Lambda_h} X_j(\omega) \varphi_j,$$

then we have $\langle u_h^\omega, \hat{A} u_h^\omega\rangle \overset{h\to 0}{\longrightarrow} L_\eta(A)$ in $L^p(\Omega)$-norm with a remainder estimate.

For example taking the Bernoulli law for the X_j then

$$u_h^\omega = \frac{1}{\sqrt{N_h}} \sum_{j\in\Lambda_h} (-1)^{\varepsilon_j(\omega)} \varphi_j$$

where $\{\varepsilon_j\}_{j\geq 1}$ are i.i.d Bernoulli variables.

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We are also able to prove that a random orthonormal basis of eigenfunctions of the Harmonic oscillator H is Quantum Uniquely Ergodic (QUE, according the terminology used in [**44**] and introduced in [**36**]).

Recall the definitions (4.3) and (4.4) of $\mathcal{B}$ and ρ. Denote by

$$B = (\varphi_{j,\ell})_{j\in\mathbb{N},\,\ell\in[\![1,N_{h_j}]\!]} \in \mathcal{B}$$

a typical orthonormal basis of $L^2(\mathbb{R}^d)$ so that for all $j \in \mathbb{N}$, $(\varphi_{j,\ell})_{\ell\in[\![1,N_{h_j}]\!]} \in U(N_{h_j})$ is an orthonormal basis of $\mathcal{E}_{h_j}$. Then

THEOREM 5.2 ([**35**], Theorem 1.6). *For $B \in \mathcal{B}$ and $A \in S(1,1)$ let us denote by*

$$D_j(B) = \max_{1\leq\ell\leq N_{h_j}} \big|\langle\varphi_{j,\ell}, \hat{A}\varphi_{j,\ell}\rangle - L_\eta(A)\big|.$$

Then we have

$$\lim_{j\to+\infty} D_j(B) = 0, \quad \rho - \text{a.s on } \mathcal{B}.$$

In other words, ρ-almost all orthonormal basis of Hermite functions is QUE.

Using estimates proved in [**6**], an analogous result to Theorem 5.2 can be proved for the Laplace operator on Riemannian compact manifolds with the same method. This holds true in particular for the sphere in any dimension $d \geq 2$ and more generally for Zoll manifolds (in this last setting a random orthonormal basis of quasi-modes is obtained).

For Schrödinger operators with super-quadratic potentials a similar result can be obtained (see [**35**]), considering orthonormal basis of quasi-modes (approximated eigenfunctions) satisfying the conclusion of Theorem 5.1.

6. Application to supercritical nonlinear Schrödinger equations

6.1. Construction of measures on $L^2(\mathbb{R}^d)$ and Strichartz inequalities. For $j \geq 1$ denote by

$$I(j) = \big\{n \in \mathbb{N},\ 2j \leq \lambda_n < 2(j+1)\big\}.$$

Observe that for all $j \geq d/2$, $I(j) \neq \emptyset$ and that $\#I(j) \sim c_d j^{d-1}$ when $j \longrightarrow +\infty$. It might also be noticed that $I(j)$ corresponds to exactly one eigenvalue λ_n of H, with multiplicity $\#I(j)$, where $\lambda_n = 2j$ if d is even and $\lambda_n = 2j+1$ if d is odd. Let us consider any fixed orthonormal basis $(\varphi_n)_{n\geq 0}$ of eigenfunctions for the harmonic oscillator H. Let $s \in \mathbb{R}$, then any $u \in \mathcal{H}^s(\mathbb{R}^d)$ can be written in a unique fashion

$$u = \sum_{j=1}^{+\infty} \sum_{n\in I(j)} c_n\varphi_n, \tag{6.1}$$

and we make the following condition on the coefficients (this is actually condition (3.2))

$$|c_k|^2 \leq \frac{C}{\#I(j)} \sum_{n\in I(j)} |c_n|^2, \quad \forall k \in I(j), \quad \forall j \geq 1. \tag{6.2}$$

We then define the random variable u^ω by

$$u^\omega = \sum_{j=1}^{+\infty} \sum_{n\in I(j)} X_n(\omega) c_n\varphi_n,$$

where $\{X_n\}_{n\geq 0}$ is a sequence of i.i.d random variables, following either the standard complex Gaussian law $\mathcal{N}_{\mathbb{C}}(0,1)$ or the Bernoulli law $\frac{1}{2}\delta_{-1}+\frac{1}{2}\delta_1$.

REMARK 6.1. *Here condition* (6.2) *allows us to use the optimal estimates on the spectral function* e_x *(see Lemma* 3.1 *and inequality* (6.3) *below). This will induce a gain of Sobolev regularity for the random series* u^ω *as it is stated in Proposition* 6.1*, compared to the deterministic Strichartz estimates* (6.4)*.*

We then have the following probabilistic improvement of the Strichartz estimates.

PROPOSITION 6.1 ([**32**], Proposition 2.1). *Let* $s\in\mathbb{R}$ *and let* $u\in\mathcal{H}^s(\mathbb{R}^d)$ *as in* (6.1)*. Assume that* $(c_n)_{n\in\mathbb{N}}$ *satisfies* (6.2)*. Let* $1\leq q<+\infty$*,* $2\leq p\leq+\infty$*, and set* $\alpha=d(1/2-1/p)$ *if* $p<+\infty$ *and* $\alpha<d/2$ *if* $p=+\infty$*. Then there exist* $c,C>0$ *so that for all* $\tau\in\mathbb{R}$

$$\mathbb{P}\left[\omega\,:\;\left\|e^{-i(t+\tau)H}u^\omega\right\|_{L^q_{[0,T]}\mathcal{W}^{s+\alpha,p}(\mathbb{R}^d)}>K\right]\leq Ce^{-\frac{cK^2}{T^{2/q}\|u\|^2_{\mathcal{H}^s(\mathbb{R}^d)}}}.$$

The first key ingredient in the proof is the Khinchin inequality (see *e.g.* [**9**, Lemma 4.2] for a proof): There exists $C>0$ such that for all real $k\geq 2$ and $(a_n)\in\ell^2(\mathbb{N})$

$$\|\sum_{n\geq 0}X_n(\omega)\,a_n\|_{L^k_{\mathbb{P}}}\leq C\sqrt{k}\Big(\sum_{n\geq 0}|a_n|^2\Big)^{\frac{1}{2}}.$$

The second key ingredient in the proof is the L^∞ estimate of the spectral function given by Thangavelu/Karadzhov (see [**33**, Lemma 3.5]) which reads for $d\geq 2$

$$\sup_{x\in\mathbb{R}}\sum_{n\in I(j)}\left|\varphi_n(x)\right|^2\leq Cj^{d/2-1}, \tag{6.3}$$

and which does not depend on the choice of the $(\varphi_n)_{n\geq 1}$.

Let us recall the deterministic Strichartz estimates for the harmonic oscillator, which can be established using the Mehler formula (see [**8**, Lemma 5.1] for the argument in 1D which can be extended). We say that a couple $(q,p)\in[2,+\infty]^2$ is admissible if

$$\frac{2}{q}+\frac{d}{p}=\frac{d}{2}\quad\text{and}\quad(d,q,p)\neq(2,2,+\infty).$$

Then for all $T>0$ there exists $C_T>0$ so that for all $u_0\in\mathcal{H}^s(\mathbb{R}^d)$ we have

$$\|\mathrm{e}^{-itH}f\|_{X^s_T}\leq C_T\|f\|_{\mathcal{H}^s(\mathbb{R}^d)}, \tag{6.4}$$

where

$$X^s_T:=\bigcap_{(q,p)\ admissible}L^q\big([-T,T]\,;\mathcal{W}^{s,p}(\mathbb{R}^d)\big).$$

When p is close to $+\infty$, the result of Proposition 6.1 expresses a gain $\mathbb{P}-$a.s. of almost $d/2$ derivatives in space compared to the bound (6.4).

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Before we state our well-posedness results, we need to define the measures on the space of initial conditions. We define the set $\mathcal{A}_s \subset \mathcal{H}^s(\mathbb{R}^d)$ by

$$\mathcal{A}_s = \Big\{ u = \sum_{j=1}^{+\infty} \sum_{n \in I(j)} c_n \varphi_n \in \mathcal{H}^s(\mathbb{R}^d) \text{ s.t. condition (6.2) holds for some } C > 0 \Big\}.$$

Let $\gamma \in \mathcal{A}_s$. We define the probability measure μ_γ on $\mathcal{H}^s$ via the map

$$\begin{aligned} \Omega &\longrightarrow \mathcal{H}^s(\mathbb{R}^d) \\ \omega &\longmapsto \gamma^\omega = \sum_{j=1}^{+\infty} \sum_{n \in I(j)} c_n X_n(\omega) \varphi_n, \end{aligned}$$

in other words, μ_γ is defined by: for all measurable $F : \mathcal{H}^s \longrightarrow \mathbb{R}$

$$\int_{\mathcal{H}^s(\mathbb{R}^d)} F(v) \mathrm{d}\mu_\gamma(v) = \int_\Omega F(\gamma^\omega) \mathrm{d}\mathbb{P}(\omega).$$

In particular, we can check that μ_γ satisfies

- If $\gamma \in \mathcal{H}^s \backslash \mathcal{H}^{s+\varepsilon}$, then $\mu_\gamma(\mathcal{H}^{s+\varepsilon}) = 0$.
- Assume that for all $j \geq 1$ such that $I(j) \neq \emptyset$ we have $c_j \neq 0$. Then for all nonempty open subset $B \subset \mathcal{H}^s$, $\mu_\gamma(B) > 0$.

Finally, we denote by $\mathcal{M}^s$ the set of all such measures

$$\mathcal{M}^s = \bigcup_{\gamma \in \mathcal{A}_s} \{\mu_\gamma\}.$$

For more properties of these measures, we refer to the introduction of [**32**].

Each element $\gamma \in \mathcal{A}_s$ defines a probability measure μ_γ. We will see in the next section that for a typical $u_0 \in \mathcal{H}^s$ in the support of μ_γ, the nonlinear Schrödinger equation with initial condition u_0 is well-posed.

By the Kakutani theorem (see also Remark 3.1), the space $\mathcal{M}^s$ contains mutually singular measures, and this extends the set of initial conditions for which we are able to solve NLS.

6.2. Application to NLS. We now consider the Cauchy problem for nonlinear Schrödinger equations, where the initial condition is random. We apply the estimates developed in the previous sections, in particular Proposition 6.1, in order to show local and global well-posedness results, for problems with Sobolev supercritical regularity.

Much work has been done on dispersive PDEs with random initial conditions since the papers of Burq-Tzvetkov [**9**, **10**]. In these articles, the authors showed that thanks to a randomisation of the initial condition one can prove well-posedness results even for data with supercritical Sobolev regularity. We also refer to [**7**, **8**, **11**, **17**, **27**, **29**–**31**, **39**] and references therein for further developments.

Let us consider nonlinear Schrödinger equation with harmonic potential

$$\begin{cases} i\dfrac{\partial u}{\partial t} + \Delta u - |x|^2 u = \pm |u|^{p-1} u, \quad (t,x) \in \mathbb{R} \times \mathbb{R}^d. \\ u(0) = u_0, \end{cases} \tag{6.5}$$

with $d \geq 2$, $p \geq 3$ an odd integer. This is a model used in the description of the Bose-Einstein condensates.

Before we state our results, let us recall some facts concerning the deterministic study of the nonlinear Schrödinger equation (6.5). We say that (6.5) is locally well-posed in $\mathcal{H}^s(\mathbb{R}^d)$, if for all initial condition $u_0 \in \mathcal{H}^s(\mathbb{R}^d)$, there exists a unique local in time solution $u \in \mathcal{C}([-T,T];\mathcal{H}^s(\mathbb{R}^d))$, and if the flow-map is uniformly continuous. We denote by

$$s_c = \frac{d}{2} - \frac{2}{p-1},$$

the critical Sobolev index. Then one can show that NLS is well-posed in $\mathcal{H}^s(\mathbb{R}^d)$ when $s > \max(s_c, 0)$, and ill-posed when $s < s_c$. We refer to the introduction of [**39**] for more details on this topic.

6.2.1. *Local existence results.* We are now able to state our first result on the local well-posedness of (6.5).

THEOREM 6.1 ([**32**], Theorem 1.1). *Let $d \geq 2$, $p \geq 3$ an odd integer and fix $\mu = \mu_\gamma \in \mathcal{M}^0$. Then there exists $\Sigma \subset L^2(\mathbb{R}^d)$ with $\mu(\Sigma) = 1$ and so that:*

(i) For all $u_0 \in \Sigma$ there exist $T > 0$ and a unique local solution u to (6.5) with initial data u_0 satisfying

$$u(t) - e^{-itH}u_0 \in \mathcal{C}\big([-T,T];\mathcal{H}^s(\mathbb{R}^d)\big), \tag{6.6}$$

for some $\frac{d}{2} - \frac{2}{p-1} < s < \frac{d}{2}$.

(ii) More precisely, for all $T > 0$, there exists $\Sigma_T \subset \Sigma$ with

$$\mu(\Sigma_T) \geq 1 - C\exp\big(-cT^{-\delta}\|\gamma\|^{-2}_{L^2(\mathbb{R}^2)}\big), \quad C, c, \delta > 0,$$

and such that for all $u_0 \in \Sigma_T$ the lifespan of u is larger than T.

Denote by $\gamma = \sum_{n=0}^{+\infty} c_n\varphi_n(x)$, then $u_0^\omega := \sum_{n=0}^{+\infty} g_n(\omega)c_n\varphi_n(x)$ is a typical element in the support of μ_γ. Another way to state Theorem 6.1 is : for any $T > 0$, there exists an event $\Omega_T \subset \Omega$ so that

$$\mathbb{P}(\Omega_T) \geq 1 - C\exp\big(-cT^{-\delta}\|\gamma\|^{-2}_{L^2(\mathbb{R}^d)}\big), \quad C, c, \delta > 0,$$

and so that for all $\omega \in \Omega_T$, there exists a unique solution of the form (6.6) to (6.5) with initial data u_0^ω.

The key argument in the proof is the use of Proposition 6.1 which yields a gain of $d/2$ derivatives compared to the deterministic theory. To prove Theorem 6.1 we only have to gain $s_c = d/2 - 2/(p-1)$ derivatives. The solution is constructed by a fixed point argument in a Strichartz space $X_T^s \subset \mathcal{C}\big([-T,T];\mathcal{H}^s(\mathbb{R}^d)\big)$ with continuous embedding, and uniqueness holds in the class X_T^s.

The deterministic Cauchy problem for (6.5) was studied by Oh [**28**] (see also Cazenave [**14**, Chapter 9] for more references). In [**39**], Thomann has proven an almost sure local existence result for (6.5) in the supercritical regime (with a gain of 1/4 of derivative), for any $d \geq 1$. This local existence result was improved by Burq-Thomann-Tzvetkov [**8**] when $d = 1$ (gain of 1/2 derivatives), by Deng [**18**] when $d = 2$, and by Poiret [**30**, **31**] in any dimension.

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6.2.2. *Global existence and scattering results for NLS.* As an application of the results of the previous part, we are able to construct global solutions to the non-linear Schrödinger equation without potential, which scatter when $t \to \pm\infty$. Consider the following equation

$$\begin{cases} i\dfrac{\partial u}{\partial t} + \Delta u = \pm|u|^{p-1}u, \quad (t,x) \in \mathbb{R}\times\mathbb{R}^d. \\ u(0) = u_0. \end{cases} \tag{6.7}$$

The well-posedness indexes for this equation are the same as for equation (6.5). Namely, (6.7) is well-posed in $H^s(\mathbb{R}^d)$ when $s > \max(s_c, 0)$, and ill-posed when $s < s_c$.

Then we can prove

THEOREM 6.2 ([**32**], Theorem 1.3). *Let $d \geq 2$, $p \geq 3$ an odd integer and fix $\mu = \mu_\gamma \in \mathcal{M}^0$. Then there exists $\Sigma \subset L^2(\mathbb{R}^d)$ with $\mu(\Sigma) > 0$ and so that:*

(i) For all $u_0 \in \Sigma$ there exists a unique global solution u to (6.7) *with initial data u_0 satisfying*

$$u(t) - e^{it\Delta}u_0 \in \mathcal{C}\big(\mathbb{R}; \mathcal{H}^s(\mathbb{R}^d)\big),$$

for some $\frac{d}{2} - \frac{2}{p-1} < s < \frac{d}{2}$.

(ii) For all $u_0 \in \Sigma$ there exist states $f_+, f_- \in \mathcal{H}^s(\mathbb{R}^d)$ so that when $t \longrightarrow \pm\infty$

$$\big\|u(t) - e^{it\Delta}(u_0 + f_\pm)\big\|_{H^s(\mathbb{R}^d)} \longrightarrow 0.$$

(iii) If we assume that the distribution of ν is symmetric, then

$$\mu\Big(u_0 \in L^2(\mathbb{R}^d) : \textit{the assertion (ii) holds true} \;\Big|\; \|u_0\|_{L^2(\mathbb{R}^d)} \leq \eta\Big) \longrightarrow 1,$$

when $\eta \longrightarrow 0$.

We can show [**31**, Théorème 20], that for all $s > 0$, if $u_0 \notin \mathcal{H}^\sigma(\mathbb{R}^d)$ then $\mu(H^\sigma(\mathbb{R}^d)) = 0$. This shows that the randomisation does not yield a gain of derivative in the Sobolev scale; thus Theorem 6.2 gives results for initial conditions which are not covered by the deterministic theory.

There is a large literature for the deterministic local and global theory with scattering for (6.7). We refer to [**2**, **12**] for such results and more references.

One of the key points in the proof is to use the lens transform $\mathscr{L}$ defined as

$$u(t,x) \longmapsto \mathscr{L}u(t,x) = \left(\frac{1}{\sqrt{1+4t^2}}\right)^{d/2} u\Big(\frac{\arctan(2t)}{2}, \frac{x}{\sqrt{1+4t^2}}\Big)\mathrm{e}^{\frac{ix^2t}{1+4t^2}},$$

which permits link equation (6.7) to equation (6.5). In particular, local in time results for (6.5) on the time interval $[-\pi/4, \pi/4]$ imply global in time results for (6.7).

In Theorem 6.2 we assumed that $d \geq 2$ and $p \geq 3$ was an odd integer, so we had $p \geq 1 + 4/d$, or in other words we were in a L^2-supercritical setting. Our approach also allows to get global in time results in an L^2-subcritical context, i.e. when $1 + 2/d < p < 1 + 4/d$.

THEOREM 6.3 ([**32**], Theorem 1.4). *Let $d = 2$ and $2 < p < 3$ and fix $\mu = \mu_\gamma \in \mathcal{M}^0$. Then there exists $\Sigma \subset L^2(\mathbb{R}^2)$ with $\mu(\Sigma) > 0$ and so that for all $0 < \varepsilon < 1$*

(i) For all $u_0 \in \Sigma$ there exists a unique global solution u to (6.7) with initial data u_0 satisfying

$$u(t) - e^{it\Delta}u_0 \in \mathcal{C}\big(\mathbb{R}; \mathcal{H}^{1-\varepsilon}(\mathbb{R}^2)\big).$$

(ii) For all $u_0 \in \Sigma$ there exist states $f_+, f_- \in \mathcal{H}^{1-\varepsilon}(\mathbb{R}^2)$ so that when $t \longrightarrow \pm\infty$

$$\big\|u(t) - e^{it\Delta}(u_0 + f_\pm)\big\|_{H^{1-\varepsilon}(\mathbb{R}^2)} \longrightarrow 0.$$

(iii) If we assume that the distribution of ν is symmetric, then

$$\mu\Big(u_0 \in L^2(\mathbb{R}^2) : \text{the assertion } (ii) \text{ holds true} \;\Big|\; \|u_0\|_{L^2(\mathbb{R}^2)} \leq \eta\Big) \longrightarrow 1,$$

when $\eta \longrightarrow 0$.

In the case $p \leq 1 + 2/d$, Barab [**3**] showed that a non trivial solution to (6.7) never scatters, therefore even with a stochastic approach one can not have scattering in this case. When $d = 2$, the condition $p > 2$ in Theorem 6.3 is therefore optimal. Usually, deterministic scattering results in L^2-subcritical contexts are obtained in the space $H^1 \cap \mathcal{F}(H^1)$. Here we assume $u_0 \in L^2$, and thus we relax both the regularity and the decay assumptions (this latter point is the most striking in this context). Again we refer to [**1**, **2**] for an overview of scattering theory for NLS.

6.2.3. *Global existence results for NLS with quadratic potential.* We also get global existence results for defocusing Schrödinger equation with harmonic potential. For $d = 2$ or $d = 3$, consider the equation

$$\begin{cases} i\dfrac{\partial u}{\partial t} - Hu = |u|^2 u, \quad (t,x) \in \mathbb{R} \times \mathbb{R}^d, \\ u(0) = u_0, \end{cases} \tag{6.8}$$

and denote by E the energy of (6.8), namely

$$E(u) = \|u\|^2_{\mathcal{H}^1(\mathbb{R}^d)} + \frac{1}{2}\|u\|^4_{L^4(\mathbb{R}^d)}.$$

Deterministic global existence for (6.8) has been studied by Zhang [**45**] and by Carles [**13**] in the case of time-dependent potentials.

When $d = 3$, our global existence result for (6.8) is the following

THEOREM 6.4 ([**32**], Theorem 1.5). *Let $d = 3$, $1/6 < s < 1$ and fix $\mu = \mu_\gamma \in \mathcal{M}^s$. Then there exists a set $\Sigma \subset \mathcal{H}^s(\mathbb{R}^3)$ so that $\mu(\Sigma) = 1$ and so that the following holds true*

(i) For all $u_0 \in \Sigma$, there exists a unique global solution to (6.8) which reads

$$u(t) = e^{-itH}u_0 + w(t), \quad w \in \mathcal{C}\big(\mathbb{R}, \mathcal{H}^1(\mathbb{R}^3)\big).$$

(ii) The previous line defines a global flow Φ, which leaves the set Σ invariant

$$\Phi(t)(\Sigma) = \Sigma, \quad \text{for all } t \in \mathbb{R}.$$

(iii) There exist $C, c_s > 0$ so that for all $t \in \mathbb{R}$,

$$E\big(w(t)\big) \leq C(M + |t|)^{c_s +},$$

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where M is a positive random variable so that

$$\mu(u_0 \in \mathcal{H}^s(\mathbb{R}^3) : M > K) \leq C e^{-\frac{cK^\delta}{\|\gamma\|^2_{\mathcal{H}^s(\mathbb{R}^3)}}}.$$

Here the critical Sobolev space is $\mathcal{H}^{1/2}(\mathbb{R}^3)$, thus the local deterministic theory combined with the conservation of the energy, immediately gives global well-posedness in $\mathcal{H}^1(\mathbb{R}^3)$. To prove Theorem 6.4, we use the high/low frequency decomposition method of Bourgain [**4**, page 84]), which relies on the almost well-posedness result of Theorem 6.1 and the global well-posedness in $\mathcal{H}^1(\mathbb{R}^3)$. As a result, we get a global well-posedness result in a supercritical context. This strategy has been successful in different contexts, and has been first used together with probabilistic arguments by Colliander-Oh [**16**] for the cubic Schrödinger below $L^2(\mathbb{S}^1)$ and later on by Burq-Tzvetkov [**11**] for the wave equation.

With a similar approach, in dimension $d = 2$, we can prove the following result

THEOREM 6.5 ([**32**], Theorem 1.6). *Let $d = 2$, $0 < s < 1$ and fix $\mu = \mu_\gamma \in \mathcal{M}^s$. Then there exists a set $\Sigma \subset \mathcal{H}^s(\mathbb{R}^2)$ so that $\mu(\Sigma) = 1$ and so that for all $u_0 \in \Sigma$, there exists a unique global solution to* (6.8) *which reads*

$$u(t) = e^{-itH}u_0 + w(t), \quad w \in \mathcal{C}\big(\mathbb{R}, \mathcal{H}^1(\mathbb{R}^2)\big).$$

In addition, statements (ii) and (iii) of Theorem 6.4 *are also satisfied with $c_s = \frac{1-s}{s}$.*

Here the critical Sobolev space is $L^2(\mathbb{R}^2)$, thus Theorem 6.5 shows global well-posedness for any subcritical cubic non linear Schrödinger equations in dimension two.

Appendix A. Proof of Theorem 3.2

LEMMA A.1. *Let $0 < \eta < 1$ and set $p_h = |\ln h|^{1-\eta}$. Then there exists a constant $C_\star = C_\star(d)$ such that*

$$(C_\star - \varepsilon/2)\sqrt{p_h} \leq \mathcal{M}_{p_h} \leq (C_\star + \varepsilon/2)\sqrt{p_h}, \tag{A.1}$$

for $h > 0$ small enough.

PROOF. In the sequel, write $p = p_h$. As in the proof of [**33**, Theorem 4.7], we denote by $\mathcal{A}_p = \mathbf{E}_h(\|u\|_{L^{p,d(p/2-1)}})^{1/p}$. Then from [**33**, estimate (4.14)] we have

$$|\mathcal{A}_p - \mathcal{M}_p| \leq CN^{-1/p}\sqrt{p} \leq \mathrm{e}^{-c|\ln h|^\eta}\sqrt{p},$$

hence it is enough to prove estimate (A.1) for $\mathcal{A}_p$. The proof then consists in tracking all the constants in [**33**] and to show that they are optimal. We do not write all the details, but we give the main steps. Let us recall [**33**, estimate (4.12)]

$$C_1\, p(c_1N)^{-p/2}\left(\int_{\mathbb{R}^d}\langle x\rangle^{d(\frac{p}{2}-1)}e_x^{p/2}\mathrm{d}x\right)\int_0^{c_0N} t^{p/2-1}\mathrm{e}^{-t}\,\mathrm{d}t \leq \mathcal{A}_p^p \leq \tag{A.2}$$
$$\leq C_2\, p(c_2N)^{-p/2}\left(\int_{\mathbb{R}^d}\langle x\rangle^{d(\frac{p}{2}-1)}e_x^{p/2}\mathrm{d}x\right)\Gamma(p/2).$$

Then for $\varepsilon > 0$

- With an inspection of the proof of [**33**, Theorem 2.6, (2.11)] and in [**33**, Lemma 2.11] we can show that we can take in the previous line
$$1/2 - \varepsilon/8 < c_2 < c_1 < 1/2 + \varepsilon/8.$$
- We can construct the parametrix in [**33**, Lemma 4.9] in such a way that
$$(\sqrt{C^\star} - \varepsilon/8)\sqrt{N} \leq \left(\int_{\mathbb{R}^d} \langle x \rangle^{d(\frac{p}{2}-1)} e_x^{p/2} \, \mathrm{d}x \right)^{1/p} \leq (\sqrt{C^\star} + \varepsilon/8)\sqrt{N},$$
where $C^\star$ is a constant which only depends on the dimension.
- With the Laplace method, we can show that for $p \geq 2$ large enough
$$(1 - \varepsilon/8)\sqrt{\frac{p}{2\mathrm{e}}} \leq \Big(\int_0^{c_0 N} t^{p/2-1} \mathrm{e}^{-t} \, \mathrm{d}t \Big)^{1/p} \leq \big(\Gamma(p/2) \big)^{1/p} \leq (1 + \varepsilon/8)\sqrt{\frac{p}{2\mathrm{e}}}.$$

Putting the previous estimates together with (A.2), we get
$$(C_\star - \varepsilon/2)\sqrt{p} \leq \mathcal{A}_p \leq (C_\star + \varepsilon/2)\sqrt{p},$$
with $C_\star = (C^\star/(2\mathrm{e}))^{1/2}$, which was the claim. □

We are now able to complete the proof of Theorem 3.2. By Lemma A.1, for $p \geq 2$ large enough
$$\Big\{ \big| \|u\|_{L^{p,d(p/2-1)}} - C_\star \sqrt{p} \big| > \varepsilon \sqrt{p} \Big\} \subset \Big\{ \Big| \|u\|_{L^{p,d(p/2-1)}} - \mathcal{M}_p \Big| > \frac{\varepsilon}{2} \sqrt{p} \Big\},$$
and an application of Theorem 3.1 gives the result.

Appendix B. Proof of Theorem 3.5

Assume here that $\delta = 1$ (the general case $0 \leq \delta \leq 1$ can be treated in the same way). To begin with, we state an estimate of $\|u\|_{L^r}$.

THEOREM B.1. *Let $2d/(d-1) < r \leq \infty$ and denote by $\mathcal{M}_r$ a median of $\|u\|_{L^r}$. Then there exist $0 < C_0 < C_1$, $K > 0$, $c_1 > 0$ and $h_0 > 0$ such that for all $r \in [2, K|\log h|]$ and $h \in]0, h_0]$ such that*
$$\mathbf{P}_{\gamma,h} \Big[u \in \mathbf{S}_h : \Big| \|u\|_{L^r} - \mathcal{M}_r \Big| > \Lambda \Big] \leq 2 \exp\big(- c_2 N_h^{2/r} h^{-\frac{d}{4}(1+\frac{2}{r})} \Lambda^2 \big).$$
and where
$$C_0 \sqrt{r} h^{\frac{d}{4}(1+\frac{2}{r})} \leq \mathcal{M}_r \leq C_1 \sqrt{r} h^{\frac{d}{4}(1-\frac{2}{r})}, \quad \forall r \in [2, K|\log h|]. \tag{B.1}$$

This is a result similar to [**33**, Theorem 4.7] in which we made the restriction $\delta < 2/3$. However, the price to pay, is that the estimate (B.1) is no more optimal. The reason is that, in this case we prove the following estimate on the spectral function when $p > d/(d-1)$ (here $r = 2p$)
$$C_0 h^{1-\frac{d}{2}(1-\frac{1}{p})} \leq \left(\int_{\mathbb{R}^d} e_x^p \, \mathrm{d}x \right)^{1/p} \leq C_1 h^{1-\frac{d}{2}(1+\frac{1}{p})}. \tag{B.2}$$

Let us prove (B.2). The upper bound is the same as in Lemma 3.1 and is proved using (2.5) (see also [**35**, Appendix A.5] for more general results). To get the lower bound, we oberve that among the family $(\varphi_j)_{j \in \Lambda_h}$ there exists a radial function $\varphi_{rad,h}$ and which satisfies $H\varphi_{rad,h} \sim \frac{1}{h}\varphi_{rad,h}$. Therefore
$$e_x := \sum_{j \in \Lambda_h} |\varphi_j|^2 \geq |\varphi_{rad,h}|^2.$$

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Now we invoke the sharp L^p bounds of radial Hermite functions, proved in [**22**, Proposition 2.4] which imply the result. Finally, to prove Theorem B.1, we proceed as in the proof of [**33**, Theorem 4.7], using the estimate (B.2).

The proof of Theorem 3.5 is analogous to [**33**, Corollary 4.8]. Roughly speaking, the L^∞ norm is reached in the regime $r = r_h = c|\ln h|$ and $h \ll 1$. In this regime, the estimate (B.1) becomes optimal, since $h^{c_1/r_h} \sim c_2$.

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Calderón problem for Maxwell's equations in the waveguide

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This paper is dedicated to the 70th birthday of Professor Jim Ralston

Abstract. For Maxwell's equations in a waveguide, we prove the global uniqueness in determination of the conductivity, the permeability and the permittivity by partial Dirichlet-to-Neumann map limited to an arbitrary subboundary.

1. Introduction and main results

Let $\widetilde{\Omega}$ be a cylinder in $\mathbf{R}^3$ and let $i = \sqrt{-1}$, $x = (x_1, x_2, x_3) \in \mathbf{R}^3$. Let $\widetilde{E} = (\widetilde{E}_1, \widetilde{E}_2, \widetilde{E}_3)$ be the electric field, $\widetilde{H} = (\widetilde{H}_1, \widetilde{H}_2, \widetilde{H}_3)$ the magnetic field, σ be the conductivity, μ the permeability and ϵ permittivity and $\omega \in \mathbf{R}^1, \omega \neq 0$ be a frequency. We set

$$\gamma = \epsilon + \frac{i\sigma}{\omega}.$$

Then Maxwell's equations are given by

$$\operatorname{curl} \widetilde{E} - i\omega\mu\widetilde{H} = 0, \quad \text{in } \widetilde{\Omega}, \tag{1.1}$$

$$\operatorname{curl} \widetilde{H} + i\omega\gamma\widetilde{E} = 0, \quad \text{in } \widetilde{\Omega}. \tag{1.2}$$

In this paper, we consider Maxwell's equation inside a waveguide $\widetilde{\Omega}$. The propagation of electromagnetic waves along waveguide is fundamentally important in electrical engineering and the modern technology is based on such propagation. As a classical book, we refer for example to Jackson [**11**], Chapter 8.

We formulate our inverse problem. Let $\Omega \subset \mathbf{R}^2$ be a bounded domain with smooth boundary $\partial\Omega$ and $\widetilde{\Omega} = \Omega \times (-\infty, \infty) = \{(x_1, x_2, x_3); (x_1, x_2) \in \Omega, x_3 \in \mathbf{R}^1\}$. We regard the x_3-direction as the longitudinal direction of a waveguide and Ω is the transverse section of the waveguide. Assume that inside the waveguide, the physical parameters μ, ϵ and σ depend only on x_1, x_2 and our inverse problem is the determination of μ, ϵ, σ by data on a part of subboundary of the waveguide. In the waveguide, the x_3-dependency of the electromagnetic field can be given by e^{hx_3}, and in a special case of $h = i\omega$ with $\omega \in \mathbf{R}^1$, the parameter ω corresponds to the frequency. In this paper, we assume

$$\widetilde{E}(x_1, x_2, x_3) = E(x_1, x_2)e^{hx_3}, \quad \widetilde{H}(x_1, x_2, x_3) = H(x_1, x_2)e^{hx_3}, \quad x_3 \in \mathbf{R}^1,$$

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where $h \in \mathbf{C}$ is a constant. Then we can rewrite Maxwell's equations in Ω:

$$L_{1,\mu,\gamma}(x,D)(E,H) := \begin{pmatrix} \partial_{x_2}E_3 - hE_2 \\ -\partial_{x_1}E_3 + hE_1 \\ \partial_{x_1}E_2 - \partial_{x_2}E_1 \end{pmatrix} - i\omega\mu \begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} = 0, \quad \text{in } \Omega, \tag{1.3}$$

and

$$L_{2,\mu,\gamma}(x,D)(E,H) := \begin{pmatrix} \partial_{x_2}H_3 - hH_2 \\ -\partial_{x_1}H_3 + hH_1 \\ \partial_{x_1}H_2 - \partial_{x_2}H_1 \end{pmatrix} + i\omega\gamma \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix} = 0, \quad \text{in } \Omega. \tag{1.4}$$

Here and henceforth we set

$$L_{\mu,\gamma}(x,D)(E,H) = (L_{1,\mu,\gamma}(x,D)(E,H), L_{2,\mu,\gamma}(x,D)(E,H)). \tag{1.5}$$

By (ν_1,ν_2) we denote the outward unit normal vector to $\partial\Omega$ and we set $\vec{\nu} = (\nu_1,\nu_2,0)$. Then we note that

$$\vec{\nu}\times E = \begin{pmatrix} \nu_2 E_3 \\ -\nu_1 E_3 \\ \nu_1 E_2 - \nu_2 E_1 \end{pmatrix} \quad \text{on } \partial\Omega. \tag{1.6}$$

Let $\widetilde{\Gamma}$ be some fixed open subset of $\partial\Omega$ and $\Gamma_0 = \partial\Omega \setminus \widetilde{\Gamma}$. Consider the following Dirichlet-to-Neumann map

$$\Lambda_{\mu,\gamma} f = \vec{\nu}\times H = \begin{pmatrix} \nu_2 H_3 \\ -\nu_1 H_3 \\ \nu_1 H_2 - \nu_2 H_1 \end{pmatrix} \quad \text{on } \widetilde{\Gamma}, \tag{1.7}$$

where

$$L_{\mu,\gamma}(x,D)(E,H) = 0 \quad \text{in } \Omega, \quad \vec{\nu}\times E|_{\Gamma_0} = 0, \quad \vec{\nu}\times E|_{\widetilde{\Gamma}} = f.$$

In general for some values of the parameter ω, the boundary value problem

$$L_{\mu,\gamma}(x,D)(E,H) = 0 \quad \text{in } \Omega, \quad \vec{\nu}\times E|_{\Gamma_0} = 0, \quad \vec{\nu}\times E|_{\widetilde{\Gamma}} = f \tag{1.8}$$

may not have a solution for some f. By $D_{\mu,\gamma}$ we denote the set of functions $f \in W_2^1(\widetilde{\Gamma})$ such that there exists at least one solution to (1.8). As for the mathematical theory of the boundary value problem for Maxwell's equations, we refer for example to Dautray and Lions [**3**].

In general for some $f \in D_{\mu,\gamma}$, there exists more than one solutions. In that case as the value of $\Lambda_{\mu,\gamma} f$, we consider the set of all functions $\vec{\nu}\times H$ where the pairs (E,H) are the all possible solutions to (1.8). Thus our definition of the Dirichlet-to-Neumann map is different from the classical one, and we have to specify the conception of the equality of the Dirichlet-to-Neumann maps.

Definition. *We say that the Dirichelt-to-Neumann maps Λ_{μ_1,γ_1} and Λ_{μ_2,γ_2} are equal if $D_{\mu_1,\gamma_1} \subset D_{\mu_2,\gamma_2}$ and for any pair (E,H) which solves*

$$L_{\mu_1,\gamma_1}(x,D)(E,H) = 0 \quad \textit{in } \Omega, \quad \vec{\nu}\times E|_{\Gamma_0} = 0, \quad \vec{\nu}\times E|_{\widetilde{\Gamma}} = f,$$

there exists a pair $(\widetilde{E},\widetilde{H})$ which solves

$$L_{\mu_2,\gamma_2}(x,D)(\widetilde{E},\widetilde{H}) = 0 \quad \textit{in } \Omega, \quad \vec{\nu}\times \tilde{E}|_{\Gamma_0} = 0, \quad \vec{\nu}\times \tilde{E}|_{\widetilde{\Gamma}} = f$$

and

$$\vec{\nu}\times H = \vec{\nu}\times \tilde{H} \quad \textit{on} \quad \widetilde{\Gamma}.$$

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Then we can state our main result:

Theorem *We assume that* $h^2+\omega^2\gamma_j\mu_j \neq 0$ *on* $\overline{\Omega}$, $j=1,2$. *Let* Ω *be a simply connected domain,* $\mu_j, \epsilon_j, \sigma_j \in C^5(\overline{\Omega})$ *for* $j\in\{1,2\}$ *and* μ_j, ϵ_j *be positive functions on* $\overline{\Omega}$. *Suppose that* $\Lambda_{\mu_1,\gamma_1}=\Lambda_{\mu_2,\gamma_2}$ *and*

$$\partial_\nu^k(\mu_1-\mu_2)=\partial_\nu^k(\gamma_1-\gamma_2)=0 \quad \text{on } \tilde{\Gamma}, \quad \forall k\in\{0,1\}. \tag{1.9}$$

Then $\mu_1=\mu_2$, $\epsilon_1=\epsilon_2$ *and* $\sigma_1=\sigma_2$ *in* Ω.

As for inverse problems by the Dirichlet-to-Neumann map for the conductivity equation, see Calderón [**1**] and Sylvester and Uhlmann [**13**] for example, and also Imanuvilov and Yamamoto [**8**] as other related results.

See Caro, Ola and Salo [**2**] and Ola, Päivärinta and Somersalo [**12**] for the uniqueness results for Maxwell's equations in three dimensions. In a special two dimensional case of $h=0$, we refer to Imanuvilov and Yamamoto [**9**], where we can reduce Maxwell's equations to the conductivity equation with zeroth order term and apply the uniqueness result in Imanuvilov, Uhlmann and Yamamoto [**5**] to prove the uniqueness.

Notations. Let $i=\sqrt{-1}$ and $\overline{z}$ be the complex conjugate of $z\in\mathbb{C}$. We set $\partial_z=\frac{1}{2}(\partial_{x_1}-i\partial_{x_2})$, $\partial_{\overline{z}}=\frac{1}{2}(\partial_{x_1}+i\partial_{x_2})$. For any holomorphic function Φ we set $\Phi'=\partial_z\Phi$ and $\overline{\Phi}'=\partial_{\overline{z}}\overline{\Phi}$, $\Phi''=\partial_z^2\Phi$,$\overline{\Phi}''=\partial_{\overline{z}}^2\overline{\Phi}$, $\vec{e}_1=(1,0),\vec{e}_2=(0,1)$. Let $\vec{\tau}=(\nu_2,-\nu_1)$ be tangential vector to $\partial\Omega$. Let $W_2^{1,\tau}(\Omega)$ be the Sobolev space $W_2^1(\Omega)$ with the norm $\|u\|_{W_2^{1,\tau}(\Omega)}=\|\nabla u\|_{L^2(\Omega)}+|\tau|\|u\|_{L^2(\Omega)}$. Moreover by $\lim_{\eta\to\infty}\frac{\|f(\eta)\|_X}{\eta}=0$ and $\|f(\eta)\|_X\leq C\eta$ as $\eta\to\infty$ with some $C>0$, we define $f(\eta)=o_X(\eta)$ and $f(\eta)=O_X(\eta)$ as $\eta\to\infty$ for a normed space X with norm $\|\cdot\|_X$, respectively. By $(\cdot,\cdot)$, we denote the scalar product in $\mathbf{R}^2$ and L^* means the adjoint of the operator L with respect to the scalar product $(\cdot,\cdot)$ in $\mathbf{R}^2$.

2. Step 1: Reduction of the Maxwell's equations to the decoupled system of elliptic equations

In this section we transform the system (1.3), (1.4) to some second order system of elliptic equation decoupled with respect to the principal part. Then we set up some new Dirichlet-to-Neumann map associated with this system of elliptic equations and show that if $\Lambda_{\mu,\gamma}$ is known, then this Dirichlet-to-Neumann map is also known. From (1.3) and (1.4) we obtain

$$\begin{aligned} H_1&=\frac{1}{i\omega\mu}(\partial_{x_2}E_3-hE_2),\\ H_2&=-\frac{1}{i\omega\mu}(\partial_{x_1}E_3-hE_1),\\ \partial_{x_1}H_2-\partial_{x_2}H_1&=-i\omega\gamma E_3 \qquad \text{in } \Omega \end{aligned} \tag{2.1}$$

and

$$\begin{aligned} E_1&=-\frac{1}{i\omega\gamma}(\partial_{x_2}H_3-hH_2),\\ E_2&=\frac{1}{i\omega\gamma}(\partial_{x_1}H_3-hH_1),\\ \partial_{x_1}E_2-\partial_{x_2}E_1&=i\omega\mu H_3 \qquad \text{in } \Omega. \end{aligned} \tag{2.2}$$

Denote $E' = (E_1, E_2), H' = (H_1, H_2)$. After we plug into the third equation of (2.1) expressions for H_1 and H_2 from the first two equations we obtain

$$\text{div}\left(\frac{1}{i\omega\mu}\nabla E_3\right) - h\text{div}\left(\frac{E'}{i\omega\mu}\right) - i\omega\gamma E_3 = 0 \quad \text{in } \Omega. \tag{2.3}$$

Similarly, from (2.2) we obtain

$$\text{div}\left(\frac{1}{i\omega\gamma}\nabla H_3\right) - h\text{div}\left(\frac{H'}{i\omega\gamma}\right) - i\omega\mu H_3 = 0 \quad \text{in } \Omega. \tag{2.4}$$

We rewrite equations (2.1) and (2.2) as

$$\begin{cases} H_1 + \frac{hE_2}{i\omega\mu} = \frac{1}{i\omega\mu}\partial_{x_2}E_3, \quad H_2 - \frac{hE_1}{i\omega\mu} = -\frac{1}{i\omega\mu}\partial_{x_1}E_3 \\ E_1 - \frac{hH_2}{i\omega\gamma} = -\frac{1}{i\omega\gamma}\partial_{x_2}H_3, \quad E_2 + \frac{hH_1}{i\omega\gamma} = \frac{1}{i\omega\gamma}\partial_{x_1}H_3. \end{cases} \tag{2.5}$$

Solving the linear system (2.5) with respect to E_1, E_2, H_1, H_2, we have

$$\begin{cases} (1 + \frac{h^2}{\omega^2\gamma\mu})E_2 = \frac{h}{\omega^2\gamma\mu}\partial_{x_2}E_3 + \frac{1}{i\omega\gamma}\partial_{x_1}H_3, \\ (1 + \frac{h^2}{\omega^2\gamma\mu})H_1 = \frac{h}{\omega^2\gamma\mu}\partial_{x_1}H_3 + \frac{1}{i\omega\mu}\partial_{x_2}E_3, \\ (1 + \frac{h^2}{\omega^2\gamma\mu})E_1 = \frac{h}{\omega^2\gamma\mu}\partial_{x_1}E_3 - \frac{1}{i\omega\gamma}\partial_{x_2}H_3, \\ (1 + \frac{h^2}{\omega^2\gamma\mu})H_2 = \frac{h}{\omega^2\gamma\mu}\partial_{x_2}H_3 - \frac{1}{i\omega\mu}\partial_{x_1}E_3. \end{cases} \tag{2.6}$$

Using the notations $g = (1 + \frac{h^2}{\omega^2\gamma\mu})$ and $\nabla^\perp P = (\frac{\partial P}{\partial x_2}, -\frac{\partial P}{\partial x_1})$, we write the above equations as

$$E' = \frac{h}{\omega^2 g\gamma\mu}\nabla E_3 - \frac{1}{i\omega\gamma g}\nabla^\perp H_3 \tag{2.7}$$

and

$$H' = \frac{h}{\omega^2 g\gamma\mu}\nabla H_3 + \frac{1}{i\omega\mu g}\nabla^\perp E_3. \tag{2.8}$$

Simple computations imply

$$\begin{aligned} h\text{div}\,(\frac{E'}{i\omega\mu}) &= \text{div}\,(\frac{h^2}{i\omega^3 g\gamma\mu^2}\nabla E_3 + \frac{h}{\omega^2\gamma\mu g}\nabla^\perp H_3) \\ &= (\nabla\frac{h^2}{i\omega^3 g\gamma\mu^2}, \nabla E_3) + (\nabla\frac{h}{\omega^2\gamma\mu g}, \nabla^\perp H_3) + \frac{h^2}{i\omega^3 g\gamma\mu^2}\Delta E_3 \end{aligned} \tag{2.9}$$

and

$$\begin{aligned} h\text{div}\,(\frac{H'}{i\omega\gamma}) &= \text{div}(\frac{h^2}{i\omega^3 g\gamma^2\mu}\nabla H_3 - \frac{h}{\omega^2\mu\gamma g}\nabla^\perp E_3) \\ &= (\nabla\frac{h^2}{i\omega^3 g\gamma^2\mu}, \nabla H_3) - (\nabla\frac{h}{\omega^2\mu\gamma g}, \nabla^\perp E_3) + \frac{h^2}{i\omega^3 g\gamma^2\mu}\Delta H_3. \end{aligned} \tag{2.10}$$

We substitute the formula for $h\text{div}\,(\frac{E'}{i\omega\mu})$ in (2.3) and the formula for $h\text{div}\,(\frac{H'}{i\omega\gamma})$ into (2.4) to obtain:

$$\begin{aligned} L_{(1)}(x, D)E_3 = \text{div}\,&\left(\left(\frac{1}{i\omega\mu} - \frac{h^2}{i\omega^3 g\gamma\mu^2}\right)\nabla E_3\right) \\ &- \left(\nabla\frac{h}{\omega^2\gamma\mu g}, \nabla^\perp H_3\right) - i\omega\gamma E_3 = 0 \quad \text{in } \Omega, \end{aligned} \tag{2.11}$$

$$E_3|_{\Gamma_0} = 0 \tag{2.12}$$

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and

$$L_{(2)}(x,D)H_3 = \operatorname{div}\left(\left(\frac{1}{i\omega\gamma} - \frac{h^2}{i\omega^3 g\gamma^2\mu}\right)\nabla H_3\right) + \left(\nabla\frac{h}{\omega^2\mu\gamma g}, \nabla^\perp E_3\right) - i\omega\mu H_3 = 0 \quad \text{in } \Omega, \tag{2.13}$$

$$\frac{\partial H_3}{\partial\nu}|_{\Gamma_0} = 0. \tag{2.14}$$

We set $\rho = (\rho_1, \rho_2, \rho_3)$ where

$$\rho_1 = \frac{1}{i\omega\mu} - \frac{h^2}{i\omega^3 g\gamma\mu^2} = \frac{\omega\gamma}{i(h^2+\omega^2\gamma\mu)}, \tag{2.15}$$

$$\rho_2 = \frac{1}{i\omega\gamma} - \frac{h^2}{i\omega^3 g\gamma^2\mu} = \frac{\omega\mu}{i(h^2+\omega^2\gamma\mu)}, \quad \rho_3 = \frac{h}{\omega^2\mu\gamma g}.$$

Then we write equations (2.11) -(2.14) as

$$L(x,D)W = \Delta W + 2A\partial_z W + 2B\partial_{\bar z}W + QW = 0 \quad \text{in } \Omega, \quad \mathcal{B}(x,D)W|_{\Gamma_0} = 0, \tag{2.16}$$

where

$$A = \begin{pmatrix} \partial_{\bar z}\ln\rho_1 & -\frac{i}{\rho_1}\partial_{\bar z}\rho_3 \\ \frac{i}{\rho_2}\partial_{\bar z}\rho_3 & \partial_{\bar z}\ln\rho_2 \end{pmatrix}, \quad B = \begin{pmatrix} \partial_z\ln\rho_1 & \frac{i}{\rho_1}\partial_z\rho_3 \\ -\frac{i}{\rho_2}\partial_z\rho_3 & \partial_z\ln\rho_2 \end{pmatrix}, \quad Q = \begin{pmatrix} \frac{-i\omega\gamma}{\rho_1} & 0 \\ 0 & \frac{-i\omega\mu}{\rho_2} \end{pmatrix}, \tag{2.17}$$

$W = (E_3, H_3)$ and $\mathcal{B}(x,D)W = (E_3, \frac{\partial H_3}{\partial\nu})$.

Indeed the equation $E_3|_{\Gamma_0} = 0$ follows from (1.6) and (1.8). Let us show that the boundary condition (2.14) holds true. By (1.6), (1.8), (2.2) and the boundary condition $\vec\nu \times E|_{\Gamma_0} = 0$ we have on Γ_0:

$$\begin{aligned} 0 = \nu_1 E_2 - \nu_2 E_1 &= \nu_1\frac{1}{i\omega\gamma}(\partial_{x_1}H_3 - hH_1) + \nu_2\frac{1}{i\omega\gamma}(\partial_{x_2}H_3 - hH_2) \\ &= \frac{1}{i\omega\gamma}(\partial_\nu H_3 - h(\vec\nu, H')). \end{aligned} \tag{2.18}$$

From (2.1) we have

$$(\vec\nu, H') = \frac{1}{i\omega\mu}\partial_{\bar\tau}E_3 - h\nu_1 E_2 + h\nu_2 E_1 = 0 \quad \text{on } \Gamma_0.$$

Hence (2.12) and (1.6), (1.8) imply (2.14).

Let us set $\mathcal{R}(x,D)W = (\partial_\nu W_1, W_2)$. Then we have

PROPOSITION 2.1. *Let the traces of the functions γ and μ be given on $\tilde\Gamma$. If the Dirichlet-to-Neumann map (1.7) is known, then the following Dirichlet-to-Neumann map is known:*

$$\mathbf{f} \to \mathcal{R}(x,D)W|_{\tilde\Gamma}, \quad L(x,D)W = 0 \quad \textit{in } \Omega, \quad \mathcal{B}(x,D)W|_{\partial\Omega} = \mathbf{f}, \quad \textit{supp}\,\mathbf{f} \subset \tilde\Gamma. \tag{2.19}$$

Proof. Let $W = (W_1, W_2)$ be a smooth function such that $L(x,D)W = 0$ in Ω. We set $E_3 = W_1$ and $H_3 = W_2$. Then we introduce functions H_1, H_2, E_1, E_2 by formulae (2.6). These formulae are equivalent to (2.7) and (2.8). Then the formulae (2.9) and (2.10) hold true. Hence we may write the equations $L_{(1)}(x,D)W = 0$ in form (2.3) and equation $L_{(2)}(x,D)W = 0$ in form (2.4). By (2.6) we have the first

two formulae in (2.1) and (2.2). Finally from the first two formulae in (2.2) and (2.4), we obtain the third formula in (2.1). Moreover from the first two formulae in (2.1) and (2.3), we obtain the third formula in (2.2). Let $\mathbf{f} = (\mathrm{f}_1, \mathrm{f}_2)$ be a smooth function, $\operatorname{supp} \mathbf{f} \subset \tilde{\Gamma}$ such that there exists a solution to the boundary value problem

$$L(x,D)W = 0 \quad \text{in } \Omega, \quad \mathcal{B}(x,D)W|_{\partial\Omega} = \mathbf{f}.$$

We set $f = (\nu_2 \mathrm{f}_1, -\nu_1 \mathrm{f}_1, \frac{1}{i\omega\gamma g}\mathrm{f}_2 - \frac{h}{\omega^2\gamma\mu g}\partial_{\bar{\tau}}\mathrm{f}_1)$. If the functions H and E are defined as above, then we have $\vec{\nu} \times E|_{\partial\Omega} = f$ and $\operatorname{supp} f \subset \tilde{\Gamma}$. Therefore $\Lambda_{\mu,\gamma} f$ is given. The formula (1.7) implies that $H_3|_{\tilde{\Gamma}} = W_2$ is given and $(\nu_1 H_2 - \nu_2 H_1)|_{\tilde{\Gamma}}$ is given. Using the formula

$$\begin{aligned}(\nu_1 H_2 - \nu_2 H_1) &= -\frac{1}{i\omega\mu}\partial_\nu E_3 + \frac{h}{i\omega\mu}(\vec{\nu}, E') \\ &= -\frac{1}{i\omega\mu}\partial_\nu E_3 + \frac{h}{\omega^2\gamma\mu}\partial_{\bar{\tau}} H_3 + \frac{h}{\omega^2\gamma\mu}(\nu_1 H_2 - \nu_2 H_1) \quad \text{on } \tilde{\Gamma}\end{aligned}$$

we obtain that $\partial_\nu E_3 = \partial_\nu W_1$ is given on $\tilde{\Gamma}$. ■

3. Step 2: Construction of the operators P_B and T_B

Let B be a 2×2 matrix with elements from $C^{5+\alpha}(\overline{\Omega})$ with $\alpha \in (0,1)$ and $\widehat{x}$ be some fixed point from Ω. By Proposition 9 of [**7**] for the equation

$$(2\partial_{\bar{z}} + B)u = 0 \quad \text{in } \Omega, \tag{3.1}$$

we can construct solutions $U_{0,k}$ such that

$$U_{0,k}(\hat{x}) = \vec{e}_k, \quad \forall k \in \{1,2\}.$$

Consider the matrix

$$\mathcal{C}(x) = (U_{0,1}(x), U_{0,2}(x)).$$

Then

$$\left(\partial_{\bar{z}} + \frac{1}{2}\mathrm{tr}B\right) \det\mathcal{C} = 0 \quad \text{in } \Omega.$$

Hence there exists a holomorphic function $q(z)$ such that $\det \mathcal{C} = q(z) e^{-\frac{1}{2}\partial_{\bar{z}}^{-1}(\mathrm{tr}\, B)}$ (see [**14**]). By $\mathcal{Q}$ we denote the set of zeros of the function q on $\overline{\Omega}$: $\mathcal{Q} = \{z \in \overline{\Omega};\, q(z) = 0\}$. Obviously $card\, \mathcal{Q} < \infty$. By κ we denote the highest order of zeros of the function q on $\overline{\Omega}$.

Using Proposition 9 of [**7**], we construct solutions $\widetilde{U}_{0,k}$ to problem (3.1) such that

$$\widetilde{U}_{0,k}(x) = \vec{e}_k \quad \forall k \in \{1,2\} \quad \text{and} \quad \forall x \in \mathcal{Q}.$$

Set $\widetilde{\mathcal{C}}(x) = (\widetilde{U}_{0,1}, \widetilde{U}_{0,2})$. Then there exists a holomorphic function $\widetilde{q}$ such that $\det \widetilde{\mathcal{C}} = \widetilde{q}(z) e^{-\frac{1}{2}\partial_{\bar{z}}^{-1}(\mathrm{tr}\, B)}$. Let $\widetilde{\mathcal{Q}} = \{z \in \overline{\Omega};\, \widetilde{q}(z) = 0\}$ and $\widetilde{\kappa}$ be the highest order of zeros of the function $\widetilde{q}$.

By $\widetilde{U}_{0,k}(x) = \vec{e_k}$ for $x \in \mathcal{Q}$, we see that

$$\widetilde{\mathcal{Q}} \cap \mathcal{Q} = \emptyset.$$

Therefore there exists a holomorphic function $r(z)$ such that

$$r|_{\mathcal{Q}} = 0 \quad \text{and} \quad (1 - r(z))|_{\widetilde{\mathcal{Q}}} = 0$$

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and the orders of zeros of the function r on $\mathcal{Q}$ and the function $1-r(z)$ on $\widetilde{\mathcal{Q}}$ are greater than or equal to $\max\{\kappa,\widetilde{\kappa}\}$.

We set

$$P_B f = \frac{1}{2}\mathcal{C}\partial_{\overline{z}}^{-1}(\mathcal{C}^{-1}rf) + \frac{1}{2}\widetilde{\mathcal{C}}\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^{-1}(1-r)f). \tag{3.2}$$

Then

$$P_B^* f = -\frac{1}{2}r(\mathcal{C}^{-1})^*\partial_{\overline{z}}^{-1}(\mathcal{C}^* f) - \frac{1}{2}(1-r)(\widetilde{\mathcal{C}}^{-1})^*\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^* f).$$

We have

PROPOSITION 3.1. *The linear operators $P_B, P_B^* \in \mathcal{L}(L^2(\Omega), W_2^1(\Omega))$ solve the differential equations*

$$(-2\partial_{\overline{z}} + B^*)P_B^* g = g, \quad (2\partial_{\overline{z}} + B)P_B g = g \quad \text{in } \Omega. \tag{3.3}$$

Proof. Since $\partial_{\overline{z}}\mathcal{C} = -\frac{1}{2}B\mathcal{C}$ and $\partial_{\overline{z}}\widetilde{\mathcal{C}} = -\frac{1}{2}B\widetilde{\mathcal{C}}$, short computations imply

$$\begin{aligned}
\partial_{\overline{z}} P_B f &= \partial_{\overline{z}}\{\frac{1}{2}\mathcal{C}\partial_{\overline{z}}^{-1}(\mathcal{C}^{-1}rf) + \frac{1}{2}\widetilde{\mathcal{C}}\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^{-1}(1-r)f)\} \\
&= \frac{1}{2}(\partial_{\overline{z}}\mathcal{C})\partial_{\overline{z}}^{-1}(\mathcal{C}^{-1}rf) + \frac{1}{2}(\partial_{\overline{z}}\widetilde{\mathcal{C}})\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^{-1}(1-r)f) \\
&\qquad + \frac{1}{2}\mathcal{C}(\mathcal{C}^{-1}rf) + \frac{1}{2}\widetilde{\mathcal{C}}(\widetilde{\mathcal{C}}^{-1}(1-r)f) \\
&= -\frac{1}{4}B\mathcal{C}\partial_{\overline{z}}^{-1}(\mathcal{C}^{-1}rf) - \frac{1}{4}B\widetilde{\mathcal{C}}\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^{-1}(1-r)f) \\
&\qquad + \frac{1}{2}rf + \frac{1}{2}(1-r)f = -\frac{1}{2}BP_B f + \frac{1}{2}f.
\end{aligned}$$

Hence the second equality in (3.3) is proved. In order to prove the first one, observe that since $\mathcal{C}\mathcal{C}^{-1}$ is the identity matrix on $\overline{\Omega}\setminus\mathcal{Q}$. The differentiation of this identity gives

$$0 = \partial_{\overline{z}}(\mathcal{C}\mathcal{C}^{-1}) = (\partial_{\overline{z}}\mathcal{C})\mathcal{C}^{-1} + \mathcal{C}\partial_{\overline{z}}\mathcal{C}^{-1} = -\frac{1}{2}B\mathcal{C}\mathcal{C}^{-1} + \mathcal{C}\partial_{\overline{z}}\mathcal{C}^{-1}.$$

This equality can be written as $\mathcal{C}\partial_{\overline{z}}\mathcal{C}^{-1} = \frac{1}{2}B$. Multiplying both sides of this equality by $\mathcal{C}^{-1}$ we have

$$\partial_{\overline{z}}\mathcal{C}^{-1} = \frac{1}{2}\mathcal{C}^{-1}B \quad \text{on} \quad \overline{\Omega}\setminus\mathcal{Q}.$$

Next we take the adjoint for the left-hand and the right-hand sides of the above equality:

$$(\partial_{\overline{z}}\mathcal{C}^{-1})^* = \partial_{\overline{z}}(\mathcal{C}^{-1})^* = (\frac{1}{2}\mathcal{C}^{-1}B)^* = \frac{1}{2}B^*(\mathcal{C}^{-1})^* \quad \text{on} \quad \overline{\Omega}\setminus\mathcal{Q}.$$

Observing that $(\mathcal{C}^{-1})^* = (\mathcal{C}^*)^{-1}$, we obtain

$$\partial_{\overline{z}}(\mathcal{C}^*)^{-1} = \frac{1}{2}B^*(\mathcal{C}^*)^{-1} \quad \text{on} \quad \overline{\Omega}\setminus\mathcal{Q}. \tag{3.4}$$

Similarly we obtain

$$\partial_{\overline{z}}(\widetilde{\mathcal{C}}^*)^{-1} = \frac{1}{2}B^*(\widetilde{\mathcal{C}}^*)^{-1} \quad \text{on} \quad \overline{\Omega}\setminus\widetilde{\mathcal{Q}}. \tag{3.5}$$

Denote by $\mathcal{C}_{ij}$ the cofactor of the i,j-element of the matrix $\mathcal{C}$ and by $\tilde{\mathcal{C}}_{ij}$ the cofactor of the i,j-element of the matrix $\tilde{\mathcal{C}}$. Setting

$$\Xi = e^{\frac{1}{2}\partial_{\overline{z}}^{-1}(\operatorname{tr} B)}\begin{pmatrix}\mathcal{C}_{11} & \mathcal{C}_{21}\\ \mathcal{C}_{12} & \mathcal{C}_{22}\end{pmatrix}, \quad \widetilde{\Xi} = e^{\frac{1}{2}\partial_{\overline{z}}^{-1}(\operatorname{tr} B)}\begin{pmatrix}\widetilde{\mathcal{C}}_{11} & \widetilde{\mathcal{C}}_{21}\\ \widetilde{\mathcal{C}}_{12} & \widetilde{\mathcal{C}}_{22}\end{pmatrix},$$

we can write the matrices $(\mathcal{C}^*)^{-1}, (\widetilde{\mathcal{C}}^*)^{-1}$ as

$$(\mathcal{C}^*)^{-1} = \frac{1}{q(z)}\Xi^* \quad \text{on} \quad \overline{\Omega}\setminus\mathcal{Q}, \quad (\widetilde{\mathcal{C}}^*)^{-1} = \frac{1}{\widetilde{q}(z)}\widetilde{\Xi}^* \quad \text{on} \quad \overline{\Omega}\setminus\widetilde{\mathcal{Q}}.$$

Then (3.4) and (3.5) imply

$$\partial_{\overline{z}}(\Xi^*)^{-1} - \frac{1}{2}B^*(\Xi^*)^{-1} = \partial_{\overline{z}}(\widetilde{\Xi}^*)^{-1} - \frac{1}{2}B^*(\widetilde{\Xi}^*)^{-1} = 0 \quad \text{on} \quad \overline{\Omega}.$$

Since r/q and $(1-r)/\widetilde{q}$ are smooth functions, the above equalities yield

$$\begin{aligned}\partial_{\overline{z}}(r(z)(\mathcal{C}^*)^{-1}) &= \frac{r(z)}{2}B^*(\mathcal{C}^*)^{-1},\\ \partial_{\overline{z}}((1-r(z))(\widetilde{\mathcal{C}}^*)^{-1}) &= \frac{1-r(z)}{2}B^*(\widetilde{\mathcal{C}}^*)^{-1} \quad \text{in} \quad \Omega.\end{aligned} \tag{3.6}$$

Using (3.6), we compute

$$\begin{aligned}\partial_{\overline{z}}P_B^*f &= -\partial_{\overline{z}}\{\frac{1}{2}r(z)(\mathcal{C}^{-1})^*\partial_{\overline{z}}^{-1}(\mathcal{C}^*f) + \frac{1}{2}(1-r(z))(\widetilde{\mathcal{C}}^{-1})^*\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^*f)\}\\ &= -\frac{1}{2}\partial_{\overline{z}}(r(z)(\mathcal{C}^{-1})^*)\partial_{\overline{z}}^{-1}(\mathcal{C}^*f) - \frac{1}{2}\partial_{\overline{z}}((1-r(z))(\widetilde{\mathcal{C}}^{-1})^*)\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^*f)\\ &\quad -\frac{1}{2}r(z)(\mathcal{C}^{-1})^*\mathcal{C}^*f - \frac{1}{2}(1-r(z))(\widetilde{\mathcal{C}}^{-1})^*\widetilde{\mathcal{C}}^*f\\ &= -\frac{1}{4}r(z)B^*(\mathcal{C}^{-1})^*\partial_{\overline{z}}^{-1}(\mathcal{C}^*f) - \frac{1}{4}(1-r(z))B^*(\widetilde{\mathcal{C}}^{-1})^*\partial_{\overline{z}}^{-1}(\widetilde{\mathcal{C}}^*f)\\ &\quad -\frac{1}{2}r(z)f - \frac{1}{2}(1-r(z))f = \frac{1}{2}B^*P_B^*f - \frac{1}{2}f.\end{aligned}$$

The proof of Proposition 3.1 is complete. ■

In a similar way we construct matrices $\mathcal{P}, \widetilde{\mathcal{P}}$, an antiholomorphic function $r_0(\overline{z})$ and operators

$$T_Bf = \frac{1}{2}\mathcal{P}\partial_z^{-1}(\mathcal{P}^{-1}r_0(\overline{z})f) + \frac{1}{2}\widetilde{\mathcal{P}}\partial_z^{-1}(\widetilde{\mathcal{P}}^{-1}(1-r_0(\overline{z}))f) \tag{3.7}$$

and

$$T_B^*f = -\frac{1}{2}r_0(\overline{z})(\mathcal{P}^{-1})^*\partial_z^{-1}(\mathcal{P}^*f) - \frac{1}{2}(1-r_0(\overline{z}))(\widetilde{\mathcal{P}}^{-1})^*\partial_z^{-1}(\widetilde{\mathcal{P}}^*f). \tag{3.8}$$

For any matrix $B \in C^{5+\alpha}(\overline{\Omega})$ with $\alpha \in (0,1)$, the linear operators T_B and T_B^* solve the differential equations

$$(2\partial_z + B)T_Bg = g \quad \text{in } \Omega; \quad (-2\partial_z + B^*)T_B^*g = g \quad \text{in } \Omega. \tag{3.9}$$

Next we introduce two operators

$$\widetilde{\mathcal{R}}_{\tau,B}g = e^{\tau(\overline{\Phi}-\Phi)}T_B(e^{\tau(\Phi-\overline{\Phi})}g), \quad \mathcal{R}_{\tau,B}g = e^{\tau(\Phi-\overline{\Phi})}P_B(e^{\tau(\overline{\Phi}-\Phi)}g). \tag{3.10}$$

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4. Step 3: Construction of complex geometric optics solutions

In this step, we will construct two complex geometric optics solutions u_1 and v respectively for operators $L_1(x,D)$ and $L_2(x,D)$.

As the phase function for such a solution, we consider a holomorphic function $\Phi(z)$ such that

$$\Phi(z) = \varphi(x_1,x_2) + i\psi(x_1,x_2)$$

with real-valued functions φ and ψ. For some $\alpha \in (0,1)$, we further assume that the function Φ belongs to $C^{6+\alpha}(\overline{\Omega})$. Moreover

$$\partial_{\overline{z}}\Phi = 0 \quad \text{in } \Omega, \quad \operatorname{Im}\Phi|_{\Gamma_0} = 0. \tag{4.1}$$

Denote by $\mathcal{H}$ the set of all the critical points of the function Φ:

$$\mathcal{H} = \{z \in \overline{\Omega};\ \Phi'(z) = 0\}.$$

Assume that Φ has no critical points on $\overline{\widetilde{\Gamma}}$, and that all critical points are nondegenerate:

$$\mathcal{H} \cap \partial\Omega = \emptyset, \quad \Phi''(z) \neq 0, \quad \forall z \in \mathcal{H}. \tag{4.2}$$

The following proposition asserts the convergence and was proved in [**8**].

PROPOSITION 4.1. *Let $\widetilde{x}$ be an arbitrary point in a simply connected domain Ω. There exists a sequence of functions $\{\Phi_\epsilon\}_{\epsilon\in(0,1)}$ satisfying (4.1), (4.2) and there exists a sequence $\{\widetilde{x}_\epsilon\}, \epsilon \in (0,1)$ such that*

$$\widetilde{x}_\epsilon \in \mathcal{H}_\epsilon = \{z \in \overline{\Omega};\ \Phi_\epsilon'(z) = 0\}, \quad \widetilde{x}_\epsilon \to \widetilde{x} \ \text{ as } \epsilon \to +0 \tag{4.3}$$

and

$$Im\,\Phi_\epsilon(\widetilde{x}_\epsilon) \notin \{Im\,\Phi_\epsilon(x);\ x \in \mathcal{H}_\epsilon \setminus \{\widetilde{x}_\epsilon\}\} \text{ and } Im\,\Phi_\epsilon(\widetilde{x}_\epsilon) \neq 0. \tag{4.4}$$

Let the function Φ satisfy (4.1), (4.2) and $\widetilde{x}$ be some point from $\mathcal{H}$. Without loss of generality, we may assume that $\widetilde{\Gamma}$ is an arc with the endpoints $x_\pm$.

Consider the following operator:

$$\begin{aligned} L_1(x,D) &= 4\partial_z\partial_{\overline{z}} + 2A_1\partial_z + 2B_1\partial_{\overline{z}} + Q_1 \\ &= (2\partial_z + B_1)(2\partial_{\overline{z}} + A_1) + Q_1(1) = (2\partial_{\overline{z}} + A_1)(2\partial_z + B_1) + Q_1(2). \end{aligned} \tag{4.5}$$

Here

$$Q_1(1) = -2\partial_z A_1 - B_1A_1 + Q_1, \quad Q_2(1) = -2\partial_{\overline{z}}B_1 - A_1B_1 + Q_1.$$

Let $U_0 = (U_{0,1}, U_{0,2}), \widetilde{U}_0 = (\tilde{U}_{0,1}, \tilde{U}_{0,2}) \in C^{6+\alpha}(\overline{\Omega})$ be a solution to the boundary value problem:

$$\mathcal{K}(x,D)(U_0,\widetilde{U}_0) = (2\partial_{\overline{z}}U_0 + A_1U_0, 2\partial_z\widetilde{U}_0 + B_1\widetilde{U}_0) = 0 \quad \text{in } \Omega, \tag{4.6}$$

$$U_0 + \mathbf{I}\widetilde{U}_0 = 0 \quad \text{on } \Gamma_0, \tag{4.7}$$

where

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We have

PROPOSITION 4.2. *Let $A_1, B_1 \in C^{5+\alpha}(\overline{\Omega})$ for some $\alpha \in (0,1)$, $\vec{r}_{0,k}, \dots, \vec{r}_{2,k} \in \mathbb{C}^3$ be arbitrary vectors and $x_1, \dots, x_k$ be mutually distinct arbitrary points from the domain Ω. There exists a solution $(U_0, \widetilde{U}_0) \in C^{6+\alpha}(\overline{\Omega})$ to problem (4.6), (4.7) such that*

$$\partial_z^j U_0(x_k) = \vec{r}_{j,k} \quad \forall j \in \{0,1,2\}, \tag{4.8}$$

$$\lim_{x \to x_\pm} \frac{|U_0(x)|}{|x - x_\pm|^{98}} = \lim_{x \to x_\pm} \frac{|\widetilde{U}_0(x)|}{|x - x_\pm|^{98}} = 0. \tag{4.9}$$

Proof. Let us fix a point $\widetilde{x}$ from $\mathcal{H} \setminus \{\widetilde{x}\}$. By Proposition 4.2 of [**6**] there exists a holomorphic function $a(z) \in C^7(\overline{\Omega})$ such that $Im\, a|_{\Gamma_0} = 0$, $a(\widetilde{x}) = 1$ and a vanishes at each point of the set $\{x_\pm\} \cup \mathcal{H} \setminus \{\widetilde{x}\}$. Let $(U_{0,0}, \widetilde{U}_{0,0}) \in C^{6+\alpha}(\overline{\Omega})$ be a solution to problem (4.6) such that $U_{0,0}(\widetilde{x}) = \vec{z}$. Since $(U_0, \widetilde{U}_0) = (a^{100} U_{0,0}, \overline{a}^{100} \widetilde{U}_{0,0})$ solves equations (4.6) and satisfies (4.7), the proof of the proposition is completed. ■

Now we start the construction of complex geometric optics solution. Let the pair $(U_0, \widetilde{U}_0)$ be defined by Proposition 4.2. Short computations and (4.5) yield

$$L_1(x,D)(U_0 e^{\tau\Phi}) = Q_1(1) U_0 e^{\tau\Phi}, \quad L_1(x,D)(\widetilde{U}_0 e^{\tau\overline{\Phi}}) = Q_1(2) \widetilde{U}_0 e^{\tau\overline{\Phi}}. \tag{4.10}$$

Let e_1, e_2 be smooth functions such that

$$e_1 + e_2 = 1 \quad \text{on } \Omega, \tag{4.11}$$

and e_1 vanishes in a neighborhood of $\partial\Omega$ and e_2 vanishes in a neighborhood of the set $\mathcal{H}$.

For any positive ϵ denote $G_\epsilon = \{x \in \Omega;\ dist(\operatorname{supp} e_1, x) > \epsilon\}$. We have

PROPOSITION 4.3. *Let $B, q \in C^{5+\alpha}(\overline{\Omega})$ for some positive $\alpha \in (0,1)$ and $\widetilde{q} \in W_p^1(\overline{\Omega})$ for some $p > 2$. Suppose that $q|_{\mathcal{H}} = \widetilde{q}|_{\mathcal{H}} = 0$. Then there exist functions $m_{\pm,\tilde{x}} \in C^2(\overline{G}_\epsilon), \tilde{x} \in \mathcal{H}$ independent of τ such that the asymptotic formulae hold true:*

$$\widetilde{\mathcal{R}}_{\tau,B}(e_1(q + \frac{\widetilde{q}}{\tau}))|_{\overline{G}_\epsilon} = e^{\tau(\overline{\Phi} - \Phi)} \left(\sum_{\tilde{x} \in \mathcal{H}} \frac{m_{+,\tilde{x}} e^{2i\tau\psi(\widetilde{x})}}{\tau^2} + o_{C^2(\overline{G}_\epsilon)}(\frac{1}{\tau^2}) \right) \ as\, |\tau| \to +\infty, \tag{4.12}$$

$$\mathcal{R}_{\tau,B}(e_1(q + \frac{\widetilde{q}}{\tau}))|_{\overline{G}_\epsilon} = e^{\tau(\Phi - \overline{\Phi})} \left(\sum_{\tilde{x} \in \mathcal{H}} \frac{m_{-,\tilde{x}} e^{-2i\tau\psi(\widetilde{x})}}{\tau^2} + o_{C^2(\overline{G}_\epsilon)}(\frac{1}{\tau^2}) \right) \ as\, |\tau| \to +\infty. \tag{4.13}$$

Denote

$$q_1 = P_{A_1}(Q_1(1) U_0) - M_1, \quad q_2 = T_{B_1}(Q_1(2) \widetilde{U}_0) - M_2 \in C^{5+\alpha}(\overline{\Omega}), \tag{4.14}$$

where the functions $M_1 \in Ker(2\partial_{\overline{z}} + A_1)$ and $M_2 \in Ker(2\partial_z + B_1)$ are taken such that

$$q_1(x) = q_2(x) = 0, \quad \forall x \in \mathcal{H}. \tag{4.15}$$

Moreover by (4.9) we can assume that

$$\lim_{x \to x_\pm} \frac{|q_1(x)|}{|x - x_\pm|^{98}} = \lim_{x \to x_\pm} \frac{|q_2(x)|}{|x - x_\pm|^{98}} = 0. \tag{4.16}$$

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Next we introduce the functions $U_{-1}, \widetilde{U}_{-1}$ as solutions to the following boundary value problem:

$$\begin{aligned} &\mathcal{K}(x,D)(U_{-1},\widetilde{U}_{-1}) = 0 \quad \text{in } \Omega, \\ &(U_{-1}+\mathbf{I}\widetilde{U}_{-1})|_{\Gamma_0} = \mathbf{I}(\frac{q_1}{2\Phi'}+\frac{q_2}{2\overline{\Phi}'}) + (0, -\frac{1}{i\partial_\nu\psi}\partial_\nu(U_0+\widetilde{U}_0,\vec{e}_2)). \end{aligned} \tag{4.17}$$

The function Φ does not have critical points on $\partial\Omega$, so does not the function ψ. Then since the tangential derivative of ψ on Γ_0 is zero, $\partial_\nu\psi$ is not zero on $\overline{\Gamma_0}$. Therefore the function $\frac{1}{i\partial_\nu\psi}$ is regular on $\overline{\Gamma_0}$.

We set $p_1 = -Q_1(2)(\frac{e_1q_1}{2\Phi'} - U_{-1}) + L_1(x,D)(\frac{e_2q_1}{2\Phi'})$, $p_2 = -Q_1(1)(\frac{e_1q_2}{2\overline{\Phi}'} - \widetilde{U}_{-1}) + L_1(x,D)(\frac{e_2q_2}{2\overline{\Phi}'})$, $\widetilde{q}_2 = T_{B_1}p_2 - \widetilde{M}_2, \widetilde{q}_1 = P_{A_1}p_1 - \widetilde{M}_1$, where $\widetilde{M}_1 \in Ker(2\partial_{\overline{z}} + A_1)$ and $\widetilde{M}_2 \in Ker(2\partial_z + B_1)$ are taken such that

$$\widetilde{q}_1(x) = \widetilde{q}_2(x) = 0, \quad \forall x \in \mathcal{H}. \tag{4.18}$$

By Proposition 4.3, there exist functions $m_{\pm,\tilde{x}} \in C^2(\overline{G}_\epsilon)$ such that

$$\begin{aligned} &\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\frac{\widetilde{q}_1}{\tau}))|_{\overline{G}_\epsilon} \\ &\quad = e^{\tau(\overline{\Phi}-\Phi)}\left(\sum_{\tilde{x}\in\mathcal{H}}\frac{m_{+,\tilde{x}}e^{2i\tau\psi(\tilde{x})}}{\tau^2} + o_{W_2^1(\overline{G}_\epsilon)}(\frac{1}{\tau^2})\right) \quad \text{as } |\tau|\to+\infty \end{aligned} \tag{4.19}$$

and

$$\begin{aligned} &\mathcal{R}_{\tau,A_1}(e_1(q_2+\frac{\widetilde{q}_2}{\tau}))|_{\overline{G}_\epsilon} \\ &\quad = e^{\tau(\Phi-\overline{\Phi})}\left(\sum_{\tilde{x}\in\mathcal{H}}\frac{m_{-,\tilde{x}}e^{-2i\tau\psi(\tilde{x})}}{\tau^2} + o_{W_2^1(\overline{G}_\epsilon)}(\frac{1}{\tau^2})\right) \quad \text{as } |\tau|\to+\infty. \end{aligned} \tag{4.20}$$

For any $\tilde{x} \in \mathcal{H}$ we introduce the functions $a_{\pm,\tilde{x}}, b_{\pm,\tilde{x}} \in C^2(\overline{\Omega})$ as solutions to the boundary value problem

$$\mathcal{K}(x,D)(a_{\pm,\tilde{x}}, b_{\pm,\tilde{x}}) = 0 \quad \text{in } \Omega, \quad (a_{\pm,\tilde{x}} + \mathbf{I}b_{\pm,\tilde{x}})|_{\Gamma_0} = m_{\pm,\tilde{x}}. \tag{4.21}$$

Let $(U_{-2}, \widetilde{U}_{-2}) \in W_2^1(\overline{\Omega})$ be a solution to the boundary value problem

$$\begin{aligned} &\mathcal{K}(x,D)(U_{-2},\widetilde{U}_{-2}) = 0 \quad \text{in } \Omega, \\ &(U_{-2}+\mathbf{I}\widetilde{U}_{-2})|_{\Gamma_0} = ((\frac{\widetilde{q}_1}{2\Phi'}+\frac{\widetilde{q}_2}{2\overline{\Phi}'},\vec{e}_1),(-\frac{\widetilde{q}_1}{2\Phi'}+\frac{\widetilde{q}_2}{2\overline{\Phi}'},\vec{e}_2)) \\ &\qquad -\frac{1}{i\partial_\nu\psi}(0,\partial_\nu(U_{-1}-\frac{e_2q_1}{2\Phi'}+\tilde{U}_{-1}-\frac{e_2q_2}{2\overline{\Phi}'},\vec{e}_2)). \end{aligned} \tag{4.22}$$

We introduce the functions $U_{0,\tau}, \widetilde{U}_{0,\tau} \in W_2^1(\Omega)$ by

$$U_{0,\tau} = U_0 + \frac{U_{-1} - e_2q_1/2\Phi'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1e_2}{2\Phi'}) \tag{4.23}$$

and

$$\widetilde{U}_{0,\tau} = \widetilde{U}_0 + \frac{\widetilde{U}_{-1} - e_2q_2/2\overline{\Phi}'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2e_2}{2\overline{\Phi}'}). \tag{4.24}$$

Simple computations and Proposition 8 of [**7**] imply for any $p \in (1,\infty)$ the asymptotic formula:

$$L_1(x,D)(-e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - \frac{e_2(q_1+\widetilde{q}_1/\tau)e^{\tau\Phi}}{2\tau\Phi'} - e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau))$$
$$-\frac{e_2(q_2+\widetilde{q}_2/\tau)e^{\tau\overline{\Phi}}}{2\tau\overline{\Phi}'}) = -L_1(x,D)(e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) + \frac{e_2(q_1+\widetilde{q}_1/\tau)e^{\tau\Phi}}{2\tau\Phi'})$$
$$-L_1(x,D)(e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)) + \frac{e_2(q_2+\widetilde{q}_2/\tau)e^{\tau\overline{\Phi}}}{2\tau\overline{\Phi}'})$$
$$= -Q_1(2)e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - Q_1(1)e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau))$$
$$-e^{\tau\Phi}L_1(x,D)(\frac{e_2(q_1+\widetilde{q}_1/\tau)}{2\tau\Phi'}) - e^{\tau\overline{\Phi}}L_1(x,D)(\frac{e_2(q_2+\widetilde{q}_2/\tau)}{2\tau\overline{\Phi}'})$$
$$-Q_1(2)\widetilde{U}_0e^{\tau\overline{\Phi}} - Q_1(1)U_0e^{\tau\Phi} + \frac{1}{\tau}(Q_1(2)(\frac{e_1q_1}{2\Phi'} - U_1) + L_1(x,D)(\frac{e_2q_1}{2\Phi'}))e^{\tau\Phi}$$
$$+\frac{1}{\tau}(Q_1(1)(\frac{e_2q_2}{2\overline{\Phi}'} - \tilde{U}_1) + L_1(x,D)(\frac{e_2q_2}{2\overline{\Phi}'}))e^{\tau\overline{\Phi}} = -\frac{1}{\tau}Q_1(2)U_{-1}e^{\tau\Phi} - \frac{1}{\tau}Q_1(1)\widetilde{U}_{-1}e^{\tau\overline{\Phi}}$$
$$-Q_1(2)\widetilde{U}_0e^{\tau\overline{\Phi}} - Q_1(1)U_0e^{\tau\Phi} + e^{\tau\varphi}o_{L^p(\Omega)}(\frac{1}{\tau}). \tag{4.25}$$

We set

$$U = U_{0,\tau}e^{\tau\Phi} + U_{0,\tau}e^{-\tau\overline{\Phi}} - e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)). \tag{4.26}$$

Using (4.25) we prove the following proposition.

PROPOSITION 4.4. *For any $p > 1$, we have the asymptotic formulae:*

$$L_1(x,D)U = e^{\tau\varphi}o_{L^p(\Omega)}(\frac{1}{\tau}) \tag{4.27}$$

and

$$\mathcal{B}(x,D)U|_{\Gamma_0} = e^{\tau\varphi}\begin{pmatrix} o_{W_2^1(\Gamma_0)}(\frac{1}{\tau^2}) \\ o_{W_2^1(\Gamma_0)}(\frac{1}{\tau}) \end{pmatrix} \quad \text{as } \tau\to\infty. \tag{4.28}$$

Proof. By (4.1), (4.19)-(4.21) and (4.17)-(4.24), we have

$$(U_{0,\tau}e^{\tau\Phi} + \widetilde{U}_{0,\tau}e^{\tau\overline{\Phi}} - e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau),\vec{e}_1)|_{\Gamma_0}$$
$$= (U_{0,\tau}e^{\tau\varphi} + \widetilde{U}_{0,\tau}e^{\tau\varphi} - e^{\tau\varphi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - e^{\tau\varphi}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)),\vec{e}_1)|_{\Gamma_0}$$
$$= e^{\tau\varphi}(U_0 + \frac{U_{-1} - e_2q_1/2\Phi'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1e_2}{2\Phi'})$$
$$+\widetilde{U}_0 + \frac{\widetilde{U}_{-1} - e_2q_2/2\overline{\Phi}'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2e_2}{2\overline{\Phi}'})$$
$$-\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - \mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau))),\vec{e}_1)|_{\Gamma_0}$$
$$= e^{\tau\varphi}(\frac{1}{\tau^2}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}} + e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}})$$
$$-\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - \mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)),\vec{e}_1)|_{\Gamma_0} = e^{\tau\varphi}o_{W_2^1(\Gamma_0)}(\frac{1}{\tau^2}).$$

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Short computations imply

$$\begin{aligned}
\mathcal{I} &= \partial_\nu(U_{0,\tau}e^{\tau\Phi} + \widetilde{U}_{0,\tau}e^{\tau\overline{\Phi}} - e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) \\
&\quad - e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau),\vec{e}_2)|_{\Gamma_0} \\
&= (i\tau\partial_\nu\psi U_{0,\tau}e^{\tau\varphi} - i\tau\partial_\nu\psi\widetilde{U}_{0,\tau}e^{\tau\varphi} + \partial_\nu U_{0,\tau}e^{\tau\varphi} + \partial_\nu\widetilde{U}_{0,\tau}e^{\tau\varphi} \\
&\quad - e^{\tau\varphi}i\partial_\nu\psi\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) + i\partial_\nu\psi e^{\tau\varphi}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)) \\
&\quad - e^{\tau\varphi}\partial_\nu\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - e^{\tau\varphi}\partial_\nu\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)),\vec{e}_2)|_{\Gamma_0} \\
&= (e^{\tau\varphi}i\tau\partial_\nu\psi(U_0 + \frac{U_{-1}-e_2q_1/2\Phi'}{\tau} \\
&\quad + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1e_2}{2\Phi'})) \\
&\quad - e^{\tau\varphi}i\tau\partial_\nu\psi(\widetilde{U}_0 + \frac{\widetilde{U}_{-1}-e_2q_2/2\overline{\Phi}'}{\tau} \\
&\quad + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2e_2}{2\overline{\Phi}'})) \\
&\quad + (e^{\tau\varphi}\partial_\nu(U_0 + \frac{U_{-1}-e_2q_1/2\Phi'}{\tau} \\
&\quad + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1e_2}{2\Phi'})) \\
&\quad + e^{\tau\varphi}\partial_\nu(\widetilde{U}_0 + \frac{\widetilde{U}_{-1}-e_2q_2/2\overline{\Phi}'}{\tau} \\
&\quad + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2e_2}{2\overline{\Phi}'})) \\
&\quad - e^{\tau\varphi}i\tau\partial_\nu\psi\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) + i\tau\partial_\nu\psi e^{\tau\varphi}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)) \\
&\quad - e^{\tau\varphi}\partial_\nu\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - e^{\tau\varphi}\partial_\nu\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)),\vec{e}_2)|_{\Gamma_0}.
\end{aligned}$$

By (4.6) and (4.17) we obtain

$$\begin{aligned}
\mathcal{I} &= (e^{\tau\varphi}i\tau\partial_\nu\psi(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1e_2}{2\Phi'})) \\
&\quad - e^{\tau\varphi}i\tau\partial_\nu\psi(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2e_2}{2\overline{\Phi}'})) \\
&\quad + (e^{\tau\varphi}\partial_\nu(\frac{U_{-1}-e_2q_1/2\Phi'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) \\
&\quad + U_{-2} - \frac{\widetilde{q}_1e_2}{2\Phi'})) + e^{\tau\varphi}\partial_\nu(\frac{\widetilde{U}_{-1}-e_2q_2/2\overline{\Phi}'}{\tau} \\
&\quad + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2e_2}{2\overline{\Phi}'})) \\
&\quad - e^{\tau\varphi}i\tau\partial_\nu\psi\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) + i\tau\partial_\nu\psi e^{\tau\varphi}\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)) \\
&\quad - e^{\tau\varphi}\partial_\nu\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1+\widetilde{q}_1/\tau)) - e^{\tau\varphi}\partial_\nu\mathcal{R}_{\tau,A_1}(e_1(q_2+\widetilde{q}_2/\tau)),\vec{e}_2)|_{\Gamma_0}.
\end{aligned}$$

Using Proposition 4.3, the formulae (4.19) and (4.20) we obtain

$$\mathcal{I} = (e^{\tau\varphi} i\tau\partial_\nu\psi(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1 e_2}{2\Phi'}))$$

$$-e^{\tau\varphi} i\tau\partial_\nu\psi(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2 e_2}{2\overline{\Phi}'}))$$

$$+(e^{\tau\varphi}\partial_\nu(\frac{U_{-1} - e_2 q_1/2\Phi'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1 e_2}{2\Phi'}))$$

$$+e^{\tau\varphi}\partial_\nu(\frac{\widetilde{U}_{-1} - e_2 q_2/2\overline{\Phi}'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2 e_2}{2\overline{\Phi}'}))$$

$$-e^{\tau\varphi} i\partial_\nu\psi\sum_{\tilde{x}\in\mathcal{H}}\frac{m_{+,\tilde{x}}e^{2i\tau\psi(\tilde{x})}}{\tau} + e^{\tau\varphi} i\partial_\nu\psi\sum_{\tilde{x}\in\mathcal{H}}\frac{m_{-,\tilde{x}}e^{-2i\tau\psi(\tilde{x})}}{\tau}$$

$$-e^{\tau\varphi}\sum_{\tilde{x}\in\mathcal{H}}\frac{\partial_\nu m_{+,\tilde{x}}e^{2i\tau\psi(\tilde{x})}}{\tau^2} - e^{\tau\varphi}\sum_{\tilde{x}\in\mathcal{H}}\frac{\partial_\nu m_{-,\tilde{x}}e^{-2i\tau\psi(\tilde{x})}}{\tau^2}, \vec{e}_2)|_{\Gamma_0} + e^{\tau\varphi} o_{W_2^1(\Gamma_0)}(\frac{1}{\tau}).$$

Using (4.22) write down $\mathcal{I}$ as

$$\mathcal{I} = (e^{\tau\varphi} i\tau\partial_\nu\psi(\frac{1}{\tau^2}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}})$$

$$-e^{\tau\varphi} i\tau\partial_\nu\psi(\frac{1}{\tau^2}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{+,\tilde{x}}))$$

$$+(e^{\tau\varphi}\partial_\nu(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1 e_2}{2\Phi'}))$$

$$+e^{\tau\varphi}\partial_\nu(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) + \widetilde{U}_{-2} - \frac{\widetilde{q}_2 e_2}{2\overline{\Phi}'}))$$

$$-e^{\tau\varphi} i\partial_\nu\psi\sum_{\tilde{x}\in\mathcal{H}}\frac{m_{+,\tilde{x}}e^{2i\tau\psi(\tilde{x})}}{\tau} + e^{\tau\varphi} i\partial_\nu\psi\sum_{\tilde{x}\in\mathcal{H}}\frac{m_{-,\tilde{x}}e^{-2i\tau\psi(\tilde{x})}}{\tau}$$

$$-e^{\tau\varphi}\sum_{\tilde{x}\in\mathcal{H}}\frac{\partial_\nu m_{+,\tilde{x}}e^{2i\tau\psi(\tilde{x})}}{\tau^2} - e^{\tau\varphi}\sum_{\tilde{x}\in\mathcal{H}}\frac{\partial_\nu m_{-,\tilde{x}}e^{-2i\tau\psi(\tilde{x})}}{\tau^2}, \vec{e}_2)|_{\Gamma_0} + e^{\tau\varphi} o_{W_2^1(\Gamma_0)}(\frac{1}{\tau}).$$

Finally, applying (4.21), we have

$$\begin{aligned}\mathcal{I} &= (e^{\tau\varphi}\partial_\nu(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}a_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}a_{-,\tilde{x}}) + U_{-2} - \frac{\widetilde{q}_1 e_2}{2\Phi'})), \vec{e}_2)|_{\Gamma_0} \\ &\quad + (e^{\tau\varphi}\partial_\nu(\frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}b_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}b_{-,\tilde{x}}) \\ &\quad + \widetilde{U}_{-2} - \frac{\widetilde{q}_2 e_2}{2\overline{\Phi}'})), \vec{e}_2)|_{\Gamma_0} + e^{\tau\varphi} o_{W_2^1(\Gamma_0)}(\frac{1}{\tau}) \\ &= e^{\tau\varphi} o_{W_2^1(\Gamma_0)}(\frac{1}{\tau}).\end{aligned}$$

The proof of equality (4.28) is complete now.

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Similarly to (4.10), using the factorization (4.5) we obtain

$$\begin{aligned} &L_1(x,D)(U_{0,\tau}e^{\tau\Phi}+\widetilde{U}_{0,\tau}e^{\tau\overline{\Phi}}+\frac{e_2(q_1+\widetilde{q}_1/\tau)e^{\tau\Phi}}{2\tau\Phi'}+\frac{e_2(q_2+\widetilde{q}_2/\tau)e^{\tau\overline{\Phi}}}{2\tau\overline{\Phi}'})\\ &=Q_1(1)(U_{0,\tau}+\frac{e_2(q_1+\widetilde{q}_1/\tau)}{2\tau\Phi'})e^{\tau\Phi}+Q_1(2)(\widetilde{U}_{0,\tau}+\frac{e_2(q_2+\widetilde{q}_2/\tau)}{2\tau\overline{\Phi}'})e^{\tau\overline{\Phi}}. \end{aligned} \tag{4.29}$$

By (4.29) and (4.25), we obtain (4.27). ■

Consider the boundary value problem

$$L(x,D)u=\Delta u+2A\partial_z u+2B\partial_{\overline{z}}u+Qu=f \quad \text{in} \quad \Omega, \quad \mathcal{B}(x,D)u|_{\partial\Omega}=0.$$

Then we prove a Carleman estimate with boundary terms whose weight function is degenerate.

PROPOSITION 4.5. *Suppose that $\Phi=\varphi+i\psi$ satisfies (4.1) and (4.2), the coefficients of the operator $L(x,D)$ matrices A,B,Q belong to $L^\infty(\Omega)$. Then there exist τ_0 and C, independent of u and τ, such that*

$$\begin{aligned} &|\tau|\|ue^{\tau\varphi}\|^2_{L^2(\Omega)}+\|ue^{\tau\varphi}\|^2_{W_2^1(\Omega)}+\tau^2\||\Phi'|ue^{\tau\varphi}\|^2_{L^2(\Omega)}\\ &\le C(\|(L(x,D)u)e^{\tau\varphi}\|^2_{L^2(\Omega)}+|\tau|\int_{\widetilde{\Gamma}}(|\nabla u|^2+\tau^2u^2)e^{2\tau\varphi}d\sigma) \end{aligned} \tag{4.30}$$

for all $|\tau|>\tau_0$ and all $u\in\{W_2^2(\Omega);\,\mathcal{B}(x,D)u|_{\Gamma_0}=0\}$.

For the scalar equation, the estimate is proved in [**5**] and [**6**] for the case of the Dirichlet and the Neumann boundary conditions respectively. In order to prove this estimate for the system, it is sufficient to apply the scalar estimate to each equation in the system and take an advantage of the large parameter in order to absorb the right-hand side.

Using estimate (4.30), we obtain

PROPOSITION 4.6. *There exists a constant τ_0 such that for $|\tau|\ge\tau_0$ and any $f\in L^2(\Omega)$, there exists a solution to the boundary value problem*

$$L(x,D+i\tau\nabla\varphi)u=f \quad \text{in } \Omega, \quad \mathcal{B}(x,D)u|_{\Gamma_0}=0 \tag{4.31}$$

such that

$$\|u\|_{W_2^{1,\tau}(\Omega)}/\sqrt{|\tau|}\le C\|f\|_{L^2(\Omega)}. \tag{4.32}$$

Moreover if $f/\Phi'\in L^2(\Omega)$, then for any $|\tau|\ge\tau_0$ there exists a solution to the boundary value problem (4.31) such that

$$\|u\|_{W_2^{1,\tau}(\Omega)}\le C\|f/\Phi'\|_{L^2(\Omega)}. \tag{4.33}$$

The constants C in (4.32) and (4.33) are independent of τ.

We set $\mathcal{O}_\epsilon=\{x\in\Omega;\,dist(x,\partial\Omega)\le\epsilon\}$. In order to construct the last term in complex geometric optics solution, we need the following proposition:

PROPOSITION 4.7. *Let $A,B\in C^{5+\alpha}(\overline{\Omega})$ and $Q\in C^{4+\alpha}(\overline{\Omega})$ for some $\alpha\in(0,1)$, $f\in L^p(\Omega)$ for some $p>2$, $dist(\overline{\Gamma}_0,supp\,f)>0$, $q\in W_2^1(\Gamma_0)$, and ϵ be a small positive number such that $\overline{\mathcal{O}_\epsilon}\cap\mathcal{H}=\emptyset$. Then there exists $C>0$ independent of τ and τ_0 such that for all $|\tau|>\tau_0$, there exists a solution $w\in W_2^1(\Omega)$ to the boundary value problem*

$$L(x,D)w=fe^{\tau\Phi} \quad \text{in } \Omega, \quad \mathcal{B}(x,D)w|_{\Gamma_0}=qe^{\tau\varphi}/\tau \tag{4.34}$$

such that

$$\sqrt{|\tau|}\|we^{-\tau\varphi}\|_{L^2(\Omega)}+\frac{1}{\sqrt{|\tau|}}\|(\nabla w)e^{-\tau\varphi}\|_{L^2(\Omega)}+\|we^{-\tau\varphi}\|_{H^{1,\tau}(\mathcal{O}_\epsilon)}\leq C(\|f\|_{L^p(\Omega)}+\|q\|_{W_2^1(\Gamma_0)}). \tag{4.35}$$

Proof. First let us assume that f is identically equal to zero. Let $(d,\widetilde{d})\in W_2^1(\Omega)\times W_2^1(\Omega)$ satisfy

$$\mathcal{K}(x,D)(d,\widetilde{d})=0 \quad \text{in}\,\Omega, \quad (d+\mathbf{I}\widetilde{d})|_{\Gamma_0}=q. \tag{4.36}$$

For the existence of such a solution see e.g., [**15**]. By (4.10) and (4.36), we have

$$L(x,D)(\frac{d}{\tau}e^{\tau\Phi}+\frac{\widetilde{d}}{\tau}e^{\tau\overline{\Phi}})=\frac{1}{\tau}(Q-2\partial_z A-BA)de^{\tau\Phi}+\frac{1}{\tau}(Q-2\partial_{\overline{z}}B-AB)\widetilde{d}e^{\tau\overline{\Phi}}.$$

By Proposition 4.6, there exists a solution w to the boundary value problem

$$L(x,D)\tilde{w}=-\frac{1}{\tau}(Q-2\partial_z A-BA)de^{\tau\Phi}-\frac{1}{\tau}(Q-2\partial_{\overline{z}}B-AB)\widetilde{d}e^{\tau\overline{\Phi}}, \quad \mathcal{B}(x,D)\tilde{w}|_{\Gamma_0}=0$$

such that there exists a constant $C>0$ such that

$$\|\tilde{w}e^{-\tau\varphi}\|_{W_2^{1,\tau}(\Omega)}\leq\frac{C}{\sqrt{|\tau|}}\|(Q-2\partial_z A-BA)de^{i\tau\psi}+(Q-2\partial_{\overline{z}}B-AB)\widetilde{d}e^{-i\tau\psi})\|_{L^2(\Omega)}$$
$$\leq\frac{C}{\sqrt{|\tau|}}\|q\|_{W_2^1(\Gamma_0)}$$

for all large $\tau>0$.

Then the function $(\frac{d}{\tau}e^{\tau\Phi}+\frac{\widetilde{d}}{\tau}e^{\tau\overline{\Phi}})+\tilde{w}$ is a solution to (4.34) which satisfies (4.35) if $f\equiv 0$.

If f is not identically equal to zero, then without loss of generality we can assume that $q\equiv 0$. Then we consider the function $\tilde{w}=\widetilde{e}e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B}(e_1q_0)$, where $\widetilde{e}\in C_0^\infty(\Omega)$, $\widetilde{e}|_{\text{supp}\,e_1}=1$, the function e_1 is defined by (4.11), $q_0=P_Af-M$, and a function $M\in C^5(\overline{\Omega})$ belongs to $Ker\,(2\partial_z+A)$ satisfying $q_0|_{\mathcal{H}}=0$. Then $L(x,D)\tilde{w}=(Q-2\partial_{\overline{z}}B-AB)\tilde{w}+\widetilde{e}e_1fe^{\tau\Phi}+2\widetilde{e}e^{\tau\Phi}q_0\partial_{\overline{z}}e_1+e^{\tau\Phi}(2\partial_{\overline{z}}+A)(\partial_z e\widetilde{\mathcal{R}}_{\tau,B}(e_1q_0))$. By Proposition 8 of [**7**], the function $\widetilde{f}(\tau,\cdot)=e^{-\tau\Phi}L(x,D)\tilde{w}-f$ can be represented as a sum of two functions where the first one is equal to zero in a neighborhood of $\mathcal{H}$ and is bounded uniformly in τ in $L^2(\Omega)$ norm and the second one is $O_{L^2(\Omega)}(\frac{1}{\tau})$. Applying Proposition 4.6 to the boundary value problem

$$L(x,D)U_*=\widetilde{f}e^{\tau\Phi} \quad \text{in}\,\Omega, \quad \mathcal{B}(x,D)U_*|_{\Gamma_0}=0,$$

we construct a solution such that

$$\|U_*e^{-\tau\varphi}\|_{W_2^{1,\tau}(\Omega)}\leq C\|f\|_{L^p(\Omega)}.$$

The function $U^*-\tilde{w}$ solves the boundary value problem (4.34) and satisfies estimate (4.35). ■

Using Propositions 4.7 and 4.4, we construct the last term u_{-1} in complex geometric optics solution which solves the equation

$$L_1(x,D)(e^{\tau\varphi}u_{-1})=-L_1(x,D)U, \quad \mathcal{B}(x,D)(e^{\tau\varphi}u_{-1})=-\mathcal{B}(x,D)U \quad \text{on}\,\Gamma_0 \tag{4.37}$$

and satisfies the estimate

$$\sqrt{|\tau|}\|u_{-1}\|_{L^2(\Omega)}+\frac{1}{\sqrt{|\tau|}}\|\nabla u_{-1}\|_{L^2(\Omega)}+\|u_{-1}\|_{W_2^{1,\tau}(\mathcal{O}_\epsilon)}=o(\frac{1}{\tau}) \quad \text{as}\,\tau\to+\infty. \tag{4.38}$$

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Finally we obtain a complex geometric optics solution in the form:

(4.39)
$$u_1(x) = U_{0,\tau}e^{\tau\Phi} + \widetilde{U}_{0,\tau}e^{\tau\overline{\Phi}} - e^{\tau\Phi}\widetilde{\mathcal{R}}_{\tau,B_1}(q_1+\widetilde{q}_1/\tau) - e^{\tau\overline{\Phi}}\mathcal{R}_{\tau,A_1}(q_2+\widetilde{q}_2/\tau) + e^{\tau\varphi}u_{-1}.$$

Obviously

$$L_1(x,D)u_1 = 0 \quad \text{in } \Omega, \quad \mathcal{B}(x,D)u_1|_{\Gamma_0} = 0. \tag{4.40}$$

Consider the operator

$$L_2(x,D)^* = 4\partial_z\partial_{\overline{z}} - 2B_2^*\partial_{\overline{z}} - 2A_2^*\partial_z + Q_2^* - 2\partial_{\overline{z}}B_2^* - 2\partial_z A_2^*$$
$$= (2\partial_z - B_2^*)(2\partial_{\overline{z}} - A_2^*) + Q_1(2) = (2\partial_{\overline{z}} - A_2^*)(2\partial_z - B_2^*) + Q_2(2).$$

Here

$$Q_1(2) = Q_2^* - 2\partial_{\overline{z}}B_2^* - B_2^*A_2^*, \quad Q_2(2) = Q_2^* - 2\partial_z A_2^* - A_2^*B_2^*.$$

Similarly we construct the complex geometric optics solutions to the operator $L_2(x,D)^*$. Let $(V_0, \widetilde{V}_0) \in C^{6+\alpha}(\overline{\Omega})\times C^{6+\alpha}(\overline{\Omega})$ be a solutions to the following boundary value problem:

(4.41)
$$\mathcal{M}(x,D)(V_0,\widetilde{V}_0) = ((2\partial_z - B_2^*)V_0, (2\partial_{\overline{z}} - A_2^*)\widetilde{V}_0) = 0 \quad \text{in } \Omega, \quad (V_0 + \mathbf{I}\widetilde{V}_0)|_{\Gamma_0} = 0,$$

such that

$$\lim_{x\to x_\pm} \frac{|V_0(x)|}{|x-x_\pm|^{98}} = \lim_{x\to x_\pm} \frac{|\widetilde{V}_0(x)|}{|x-x_\pm|^{98}} = 0. \tag{4.42}$$

Such a pair $(V_0, \widetilde{V}_0)$ exists due to Proposition 4.2. Observe that

$$L_2(x,D)^*(\widetilde{V}_0 e^{-\tau\Phi}) = Q_1(2)\widetilde{V}_0 e^{-\tau\Phi} \quad \text{in } \Omega,$$
$$L_2(x,D)^*(V_0 e^{-\tau\overline{\Phi}}) = Q_2(2)V_0 e^{-\tau\overline{\Phi}} \quad \text{in } \Omega.$$

We set

$$q_3 = P_{-A_2^*}(Q_1(2)\widetilde{V}_0) - M_3, \quad q_4 = T_{-B_2^*}(Q_2(2)V_0) - M_4, \tag{4.43}$$

where $M_3 \in Ker(2\partial_{\overline{z}} - A_2^*)$ and $M_4 \in Ker(2\partial_z - B_2^*)$ are chosen such that

$$q_3(x) = q_4(x) = 0, \quad \forall x \in \mathcal{H} \quad \text{and} \lim_{x\to x_\pm} \frac{|q_j(x)|}{|x-x_\pm|^{98}} = 0 \quad j \in \{3,4\}. \tag{4.44}$$

By (4.44) the functions $\frac{q_3}{2\Phi'}$ and $\frac{q_4}{2\overline{\Phi}'}$ belong to $C^2(\overline{\Gamma}_0)$. Therefore we can introduce the functions $V_{-1}, \widetilde{V}_{-1}$ as solutions to the following boundary value problem:

$$\begin{aligned} &\mathcal{M}(x,D)(V_{-1},\widetilde{V}_{-1}) = 0 \quad \text{in } \Omega, \\ &(V_{-1} + \mathbf{I}\widetilde{V}_{-1})|_{\Gamma_0} = -(\mathbf{I}\frac{q_3}{2\Phi'} + \frac{q_4}{2\overline{\Phi}'}) - (0, (\vec{e}_2, B(x,D)^*(V_0+\tilde{V}_0))/i\partial_\nu\psi). \end{aligned} \tag{4.45}$$

Let

$$p_3 = Q_1(2)(\frac{e_1 q_3}{2\Phi'} + \widetilde{V}_{-1}) + L_2(x,D)^*(\frac{q_3 e_2}{2\Phi'}),$$
$$p_4 = Q_2(2)(\frac{e_1 q_4}{2\overline{\Phi}'} + V_{-1}) + L_2(x,D)^*(\frac{q_4 e_2}{2\overline{\Phi}'})$$

and

$$\widetilde{q}_4 = (T_{-B_2^*}p_4 - \widetilde{M}_3), \quad \widetilde{q}_3 = (P_{-A_2^*}p_3 - \widetilde{M}_4),$$

where $\widetilde{M}_3 \in Ker(2\partial_z - B_2^*), \widetilde{M}_4 \in Ker(2\partial_{\overline{z}} - A_2^*)$, and $(\widetilde{q}_3, \widetilde{q}_4)$ are chosen such that

$$\widetilde{q}_3(x) = \widetilde{q}_4(x) = 0, \quad \forall x \in \mathcal{H}. \tag{4.46}$$

The following asymptotic formula holds true:

PROPOSITION 4.8. *There exist smooth functions* $\widetilde{m}_{\pm,\tilde{x}} \in C^2(\overline{G}_\epsilon), \tilde{x} \in \mathcal{H}$, *independent of* τ *such that*

$$\widetilde{\mathcal{R}}_{-\tau,-B_2^*}(e_1(q_3+\widetilde{q}_3/\tau))|_{\overline{G}_\epsilon} = \sum_{\tilde{x}\in\mathcal{H}} \frac{\widetilde{m}_{+,\tilde{x}} e^{2i\tau(\psi-\psi(\tilde{x}))}}{\tau^2} + e^{2i\tau\psi} o_{W_2^1(\partial\Omega)}(\frac{1}{\tau^2}) \quad as\ |\tau|\to+\infty \tag{4.47}$$

and

$$\mathcal{R}_{-\tau,-A_2^*}(e_1(q_4+\widetilde{q}_4/\tau))|_{\overline{G}_\epsilon} = \sum_{\tilde{x}\in\mathcal{H}} \frac{\widetilde{m}_{-,\tilde{x}} e^{-2i\tau(\psi-\psi(\tilde{x}))}}{\tau^2} + e^{-2i\tau\psi} o_{W_2^1(\partial\Omega)}(\frac{1}{\tau^2}) \quad as\ |\tau|\to+\infty. \tag{4.48}$$

Using the functions $\tilde{m}_{\pm,\tilde{x}}$ we introduce functions $\widetilde{a}_{\pm,\tilde{x}}, \widetilde{b}_{\pm,\tilde{x}} \in C^2(\overline{\Omega})$ which solve the boundary value problem

$$\mathcal{M}(x,D)(\widetilde{a}_{\pm,\tilde{x}}, \widetilde{b}_{\pm,\tilde{x}}) = 0 \quad \text{in } \Omega, \quad (\widetilde{a}_{\pm,\tilde{x}} + \mathbf{I}\widetilde{b}_{\pm,\tilde{x}})|_{\Gamma_0} = -\widetilde{m}_{\pm,\tilde{x}} \quad \forall \tilde{x}\in\mathcal{H}. \tag{4.49}$$

By (4.46), there exists a pair $(V_{-2}, \widetilde{V}_{-2}) \in W_2^1(\Omega)\times W_2^1(\Omega)$ which solves the boundary value problem

$$\mathcal{M}(x,D)(V_{-2}, \widetilde{V}_{-2}) = 0 \quad \text{in } \Omega, \tag{4.50}$$

$$(V_{-2}+\mathbf{I}\widetilde{V}_{-2})|_{\Gamma_0} = -(\mathbf{I}\frac{\widetilde{q}_3}{2\Phi'}+\frac{\widetilde{q}_4}{2\overline{\Phi}'})-(0,\vec{e}_2,B(x,D)^*(\tilde{V}_{-1}+\frac{e_2q_3}{2\Phi'}+V_{-1}+\frac{e_2q_4}{2\overline{\Phi}'}))/i\partial_\nu\psi). \tag{4.51}$$

We introduce functions $V_{0,\tau}, \widetilde{V}_{0,\tau}$ by formulae

$$\tilde{V}_{0,\tau} = \tilde{V}_0 + \frac{\tilde{V}_{-1}+\frac{e_2q_3}{2\Phi'}}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}\widetilde{b}_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}\widetilde{b}_{-,\tilde{x}}) + \tilde{V}_{-2} + \frac{e_2\widetilde{q}_3}{2\Phi'}) \tag{4.52}$$

and

$$V_{0,\tau} = V_0 + \frac{V_{-1}+e_2q_4/2\overline{\Phi}'}{\tau} + \frac{1}{\tau^2}(\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}\widetilde{a}_{+,\tilde{x}} + e^{-2i\tau\psi(\tilde{x})}\widetilde{a}_{-,\tilde{x}}) + V_{-2} + \frac{e_2\widetilde{q}_4}{2\overline{\Phi}'}). \tag{4.53}$$

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By (4.44) and (4.46), the functions $V_{0,\tau}, \widetilde{V}_{0,\tau}$ belong to $W_2^1(\Omega)$. After short computations, for any $p \in (1, +\infty)$ we have

$$\begin{aligned}
&L_2(x,D)^* \left(-e^{-\tau\Phi}\widetilde{\mathcal{R}}_{-\tau,-B_2^*}(e_1(q_3+\frac{\widetilde{q}_3}{\tau})) + \frac{e^{-\tau\Phi}e_2(q_3+\frac{\widetilde{q}_3}{\tau})}{2\tau\Phi'} \right. \\
&\qquad \left. -e^{-\tau\overline{\Phi}}\mathcal{R}_{-\tau,-A_2^*}(e_1(q_4+\frac{\widetilde{q}_4}{\tau})) + \frac{e^{-\tau\overline{\Phi}}e_2(q_4+\frac{\widetilde{q}_4}{\tau})}{2\tau\overline{\Phi}'} \right) \\
&= -e^{-\tau\Phi}Q_2(2)\widetilde{\mathcal{R}}_{-\tau,-B_2^*}(e_1(q_3+\frac{\widetilde{q}_3}{\tau})) + e^{-\tau\Phi}L_2(x,D)^*(\frac{e_2(q_3+\frac{\widetilde{q}_3}{\tau})}{2\tau\Phi'}) \\
&\quad - e^{-\tau\overline{\Phi}}(Q_1(2)\mathcal{R}_{-\tau,-A_2^*}(e_1(q_4+\frac{\widetilde{q}_4}{\tau})) + e^{-\tau\overline{\Phi}}L_2(x,D)^*(\frac{e_2(q_4+\frac{\widetilde{q}_4}{\tau})}{2\tau\overline{\Phi}'}) \\
&\quad - e^{-\tau\Phi}Q_2(2)\frac{e_1q_3}{2\tau\Phi'} - e^{-\tau\overline{\Phi}}Q_1(2)\frac{e_1q_4}{2\tau\overline{\Phi}'} - e^{-\tau\Phi}L_2(x,D)^*(\frac{e_2q_3}{2\tau\Phi'}) \\
&\quad - e^{-\tau\overline{\Phi}}L_2(x,D)^*(\frac{e_2q_4}{2\tau\overline{\Phi}'}) \\
&\quad - Q_1(2)(\tilde{V}_{-1}+\frac{\tilde{V}_{-2}}{\tau})e^{-\tau\Phi} - Q_2(2)(V_{-1}+\frac{V_{-2}}{\tau})e^{-\tau\overline{\Phi}} \\
&= -Q_1(2)(\tilde{V}_{-1}+\frac{\tilde{V}_{-2}}{\tau})e^{-\tau\Phi} - Q_2(2)(V_{-1}+\frac{V_{-2}}{\tau})e^{-\tau\overline{\Phi}} + e^{-\tau\varphi}o_{L^p(\Omega)}(\frac{1}{\tau}). \qquad (4.54)
\end{aligned}$$

Setting

$$V^* = V_{0,\tau}e^{-\tau\overline{\Phi}} + \widetilde{V}_{0,\tau}e^{-\tau\Phi} - e^{-\tau\Phi}\widetilde{\mathcal{R}}_{-\tau,-B_2^*}(e_1(q_3+\frac{\widetilde{q}_3}{\tau})) - e^{-\tau\overline{\Phi}}\mathcal{R}_{-\tau,-A_2^*}(e_1(q_4+\frac{\widetilde{q}_4}{\tau})) \qquad (4.55)$$

for any $p \in (1,\infty)$, we obtain that

$$L_2(x,D)^*V^* = e^{-\tau\varphi}o_{L^p(\Omega)}(\frac{1}{\tau}) \quad \text{in } \Omega, \quad \mathcal{B}^*(x,D)V^*|_{\Gamma_0} = e^{-\tau\varphi}\begin{pmatrix} o_{W_2^1(\Gamma_0)}(\frac{1}{\tau^2}) \\ o_{W_2^1(\Gamma_0)}(\frac{1}{\tau}) \end{pmatrix}. \qquad (4.56)$$

The first equality in (4.56) follows from (4.54) and the second one can be obtained by argument similar to one used in the proof of Proposition 4.4.

Using (4.56) and Proposition 4.7, we construct the last term v_{-1} by a complex geometric optics solution which solves the boundary value problem

$$L_2(x,D)^*v_{-1} = -L_2(x,D)^*V^* \quad \text{in } \Omega, \quad \mathcal{B}(x,D)^*v_{-1}|_{\Gamma_0} = -\mathcal{B}(x,D)^*V^* \qquad (4.57)$$

and satisfies the estimate

$$\sqrt{|\tau|}\|v_{-1}\|_{L^2(\Omega)} + \frac{1}{\sqrt{|\tau|}}\|\nabla v_{-1}\|_{L^2(\Omega)} + \|v_{-1}\|_{W_2^{1,\tau}(\mathcal{O}_\epsilon)} = o(\frac{1}{\tau}) \quad \text{as } \tau \to +\infty. \qquad (4.58)$$

Finally we have a complex geometric optics solution for the Schrödinger operator $L_2(x,D)^*$ in a form:

$$\begin{aligned}
v = V_{1,\tau}e^{-\tau\overline{\Phi}} + \widetilde{V}_{1,\tau}e^{-\tau\Phi} - e^{-\tau\Phi}\widetilde{\mathcal{R}}_{-\tau,-B_2^*}(e_1(q_3+\frac{\widetilde{q}_3}{\tau})) \\
-e^{-\tau\overline{\Phi}}\mathcal{R}_{-\tau,-A_{2,}^*}(e_1(q_4+\frac{\widetilde{q}_4}{\tau})) + v_{-1}e^{-\tau\varphi}.
\end{aligned} \qquad (4.59)$$

By (4.59) and (4.57), we have

$$L_2(x,D)^*v = 0 \quad \text{in } \Omega, \quad \mathcal{B}(x,D)^*v|_{\Gamma_0} = 0. \qquad (4.60)$$

5. Step 4: Asymptotics

We introduce the following functionals

$$\mathfrak{F}_{\tau,\tilde{x}}u = \frac{\pi}{2|\det \psi''(\tilde{x})|^{\frac{1}{2}}} \times \left(\frac{u(\widetilde{x})}{\tau} - \frac{\partial^2_{zz}u(\widetilde{x})}{2\Phi''(\tilde{x})\tau^2} + \frac{\partial^2_{\overline{z}\overline{z}}u(\widetilde{x})}{2\overline{\Phi}''(\tilde{x})\tau^2} + \frac{(\partial_z u(\widetilde{x}))\Phi'''(\tilde{x})}{2(\Phi''(\tilde{x}))^2\tau^2} - \frac{(\partial_{\overline{z}} u(\widetilde{x}))\overline{\Phi}'''(\tilde{x})}{2(\overline{\Phi}''(\tilde{x}))^2\tau^2} \right)$$

and

$$\mathfrak{I}_\tau u = \int_{\partial\Omega} u \frac{\nu_1 - i\nu_2}{2\tau\Phi'} e^{\tau(\Phi-\overline{\Phi})} d\sigma - \int_{\partial\Omega} \frac{\nu_1 - i\nu_2}{\Phi'} \partial_z \left(\frac{u}{2\tau^2\Phi'} \right) e^{\tau(\Phi-\overline{\Phi})} d\sigma.$$

Using these notations and the fact that Φ is a harmonic function, we rewrite the classical result of theorem 7.7.5 of [**4**] as

PROPOSITION 5.1. *Let $\Phi(z)$ satisfy (4.1), (4.2) and let $u \in C^{5+\alpha}(\Omega)$ with $\alpha \in (0,1)$. Then*

$$\int_\Omega u e^{\tau(\Phi-\overline{\Phi})} dx = \sum_{\tilde{x}\in\mathcal{H}} e^{2i\tau\psi(\tilde{x})} \mathfrak{F}_{\tau,\tilde{x}}u + \mathfrak{I}_\tau u + o\left(\frac{1}{\tau}\right) \quad \text{as } \tau \to +\infty. \tag{5.1}$$

Denote

$$\mathbf{H}(x, \partial_z, \partial_{\overline{z}}) = 2\mathcal{A}\partial_z + 2\mathcal{B}\partial_{\overline{z}} + \mathcal{Q},$$

where $\mathcal{A}(x) = A_1 - A_2, \mathcal{B}(x) = B_1 - B_2$ and $\mathcal{Q}(x) = Q_1 - Q_2$. We have

PROPOSITION 5.2. *Suppose that for any U given by (4.23), (4.24), (4.26) and V^* given by (4.52), (4.53), (4.55) with any function Φ which satisfies (4.1) and (4.2), we have*

$$\mathcal{J}_\tau = \int_\Omega (\mathbf{H}(x, \partial_z, \partial_{\overline{z}})U, V^*) dx = o(\frac{1}{\tau}) \quad \text{as } \tau \to +\infty.$$

Then there exist constants J_k independent of τ such that

$$\begin{aligned} \mathcal{J}_\tau = &\sum_{k=-1}^{1} \tau^k J_k + \frac{1}{\tau} \sum_{\tilde{x}\in\mathcal{H}} ((J_+ + I_{+,\Phi} + K_+)(\tilde{x}) e^{2\tau i\psi(\tilde{x})} \\ &+ (J_- + I_{-,\Phi} + K_-)(\tilde{x}) e^{-2\tau i\psi(\tilde{x})}) \\ &+ \int_{\tilde{\Gamma}} ((\nu_1 - i\nu_2)(\mathcal{A}U_0 e^{\tau\Phi}, V_0 e^{-\tau\overline{\Phi}}) + (\nu_1 + i\nu_2)(\mathcal{B}\tilde{U}_0 e^{\tau\overline{\Phi}}, \tilde{V}_0 e^{-\tau\Phi})) d\sigma \\ &+ o(\frac{1}{\tau}) \quad \text{as } \tau \to +\infty, \end{aligned} \tag{5.2}$$

where

$$J_+(\tilde{x}) = \frac{\pi}{|det\, \psi''(\tilde{x})|^{\frac{1}{2}}} (-(2\partial_z \mathcal{A}U_0, V_0) - (\mathcal{A}U_0, B_2^* V_0) - (\mathcal{B}A_1 U_0, V_0) + (\mathcal{Q}U_0, V_0))(\tilde{x}), \tag{5.3}$$

$$J_-(\tilde{x}) = \frac{\pi}{|det\, \psi''(\tilde{x})|^{\frac{1}{2}}} (-(2\mathcal{A}B_1 \tilde{U}_0, \tilde{V}_0) - (2\partial_{\overline{z}} \mathcal{B}\tilde{U}_0, \tilde{V}_0) - (\mathcal{B}\tilde{U}_0, A_2^* \tilde{V}_0)) + (\mathcal{Q}\tilde{U}_0, \tilde{V}_0))(\tilde{x}), \tag{5.4}$$

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$$I_{+,\Phi}(\tilde{x}) = -\int_{\partial\Omega}\Big\{(\nu_1 - i\nu_2)((2b_{+,\tilde{x}}\overline{\Phi}', V_0) + (2\overline{\Phi}'U_0, \tilde{a}_{+,\tilde{x}})) \\ +(\nu_1 + i\nu_2)((2a_{+,\tilde{x}}\Phi', \tilde{V}_0) + (2\Phi'\tilde{U}_0, \tilde{b}_{+,\tilde{x}}))\Big\}\, d\sigma, \tag{5.5}$$

$$I_{-,\Phi}(\tilde{x}) = -\int_{\partial\Omega}\Big\{(\nu_1 - i\nu_2)((2b_{+,\tilde{x}}\overline{\Phi}', V_0) + (2\overline{\Phi}'U_0, \tilde{a}_{+,\tilde{x}})) \\ +(\nu_1 + i\nu_2)((2a_{+,\tilde{x}}\Phi', \tilde{V}_0) + (2\Phi'\tilde{U}_0, \tilde{b}_{+,\tilde{x}}))\Big\}\, d\sigma, \tag{5.6}$$

$$K_+ = \tau\mathfrak{F}_{\tau,\tilde{x}}(q_1, T^*_{B_1}(B_1^*\mathcal{A}^*V_0) - \mathcal{A}^*V_0 + 2T^*_{B_1}(\partial_z\mathcal{B}^*V_0) + T^*_{B_1}(\mathcal{B}^*(A_2^*V_0 - 2\tau\overline{\Phi}'V_0))) \\ -2\tau\mathfrak{F}_{\tau,\tilde{x}}(P^*_{-A_2^*}(\mathcal{A}(\partial_z U_0 + \tau\Phi'U_0) + \mathcal{B}\partial_{\overline{z}}U_{0,\tau}), q_4). \tag{5.7}$$

Proof. Denote

$$U_1 = -\widetilde{\mathcal{R}}_{\tau,B_1}(e_1(q_1 + \widetilde{q}_1/\tau)), \quad \tilde{U}_1 = -\mathcal{R}_{\tau,A_1}(e_1(q_2 + \widetilde{q}_2/\tau)), \tag{5.8}$$

$$\tilde{V}_1 = -\widetilde{\mathcal{R}}_{-\tau,-B_2^*}(e_1(q_3 + \widetilde{q}_3/\tau)), \quad V_1 = -\mathcal{R}_{-\tau,-A_2^*}(e_1(q_4 + \widetilde{q}_4/\tau)). \tag{5.9}$$

Integrating by parts and using Proposition 5.1, we obtain

$$\begin{aligned}
\mathcal{M}_1 &:= \int_\Omega (2\mathcal{A}\partial_z(U_{0,\tau}e^{\tau\Phi}) + 2\mathcal{B}\partial_{\overline{z}}(U_{0,\tau}e^{\tau\Phi}), V_{0,\tau}e^{-\tau\overline{\Phi}})dx \\
&= \int_\Omega ((-2\partial_z\mathcal{A}U_{0,\tau}e^{\tau\Phi}, V_{0,\tau}e^{-\tau\overline{\Phi}}) \\
&\quad - (2\mathcal{A}U_{0,\tau}e^{\tau\Phi}, \partial_z V_{0,\tau}e^{-\tau\overline{\Phi}}) + (2\mathcal{B}\partial_{\overline{z}}U_{0,\tau}e^{\tau\Phi}, V_{0,\tau}e^{-\tau\overline{\Phi}}))dx \\
&\quad + \int_{\partial\Omega}(\nu_1 - i\nu_2)(\mathcal{A}U_{0,\tau}e^{\tau\Phi}, V_{0,\tau}e^{-\tau\overline{\Phi}})d\sigma \\
&= \sum_{\tilde{x}\in\mathcal{H}} e^{2i\tau\psi(\tilde{x})}\mathfrak{F}_{\tau,\tilde{x}}(-(2\partial_z\mathcal{A}U_0, V_0) - (2\mathcal{A}U_0, \partial_z V_0) + (2\mathcal{B}\partial_{\overline{z}}U_0, V_0)) \\
&\quad + \mathfrak{I}_\tau(-(2\partial_z\mathcal{A}U_{0,\tau}, V_{0,\tau}) - (2\mathcal{A}U_{0,\tau}, \partial_z V_{0,\tau}) + (2\mathcal{B}\partial_{\overline{z}}U_{0,\tau}, V_{0,\tau})) \\
&\quad + \int_{\tilde{\Gamma}}(\nu_1 - i\nu_2)(\mathcal{A}U_0, V_0)e^{\tau(\Phi-\overline{\Phi})}d\sigma + \kappa_{0,0} + \frac{\kappa_{0,-1}}{\tau} + o(\frac{1}{\tau}),
\end{aligned} \tag{5.10}$$

where $\kappa_{0,j}$ are some constants independent of τ.

Integrating by parts we obtain that there exist constants $\kappa_{1,j}$ independent of τ such that

(5.11)

$$\begin{aligned}
&\int_\Omega (2\mathcal{A}\partial_z(\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}) + 2\mathcal{B}\partial_{\overline{z}}(\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}), V_{0,\tau}e^{-\tau\overline{\Phi}})dx \\
&= (2\mathcal{A}\partial_z\tilde{U}_{0,\tau}, V_{0,\tau})_{L^2(\Omega)} + (2\mathcal{B}(\partial_z\tilde{U}_{0,\tau} + \tau\overline{\Phi}'\tilde{U}_{0,\tau}), V_{0,\tau})_{L^2(\Omega)} \\
&= \tau\kappa_{1,1} + \kappa_{1,0} + \frac{\kappa_{1,-1}}{\tau} + \frac{1}{\tau}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}(2\mathcal{B}b_{+,\tilde{x}}\overline{\Phi}', V_0)_{L^2(\Omega)} \\
&\quad + e^{-2i\tau\psi(\tilde{x})}(2\mathcal{B}b_{-,\tilde{x}}\overline{\Phi}', V_0)_{L^2(\Omega)}) \\
&\quad + \frac{1}{\tau}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}(2\mathcal{B}\overline{\Phi}'U_0, \tilde{a}_{+,\tilde{x}})_{L^2(\Omega)} + e^{-2i\tau\psi(\tilde{x})}(2\mathcal{B}\overline{\Phi}'U_0, \tilde{a}_{-,\tilde{x}})_{L^2(\Omega)}) + o(\frac{1}{\tau}).
\end{aligned}$$

Since by (4.6), (4.21), (4.41) and (4.49) we have

$$-(2\mathcal{B}\overline{\Phi}'U_0,\tilde{a}_{\pm,\tilde{x}})=4\partial_z(\overline{\Phi}'U_0,\tilde{a}_{\pm,\tilde{x}}),\ \text{and}\ -(2\mathcal{B}b_{\pm,\tilde{x}}\overline{\Phi}',V_0)=4\partial_z(b_{\pm,\tilde{x}}\overline{\Phi}',V_0)\ \text{in}\ \Omega$$

for any $\tilde{x}$ from $\mathcal{H}$, from (5.11) we have

(5.12)

$$\begin{aligned}\mathcal{M}_2 &:= \int_\Omega (2\mathcal{A}\partial_z(\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}})+2\mathcal{B}\partial_{\overline{z}}(\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}),V_{0,\tau}e^{-\tau\overline{\Phi}})dx\\ &= \tau\kappa_{1,1}+\kappa_{1,0}+\frac{\kappa_{1,-1}}{\tau}\\ &\quad -\int_{\partial\Omega}\sum_{\tilde{x}\in\mathcal{H}}\frac{\nu_1-i\nu_2}{\tau}(e^{2i\tau\psi(\tilde{x})}(2\mathcal{B}b_{+,\tilde{x}}\overline{\Phi}',V_0)+e^{-2i\tau\psi(\tilde{x})}(2\mathcal{B}b_{-,\tilde{x}}\overline{\Phi}',V_0))d\sigma\\ &\quad -\int_{\partial\Omega}\sum_{\tilde{x}\in\mathcal{H}}\frac{\nu_1-i\nu_2}{\tau}(e^{2i\tau\psi(\tilde{x})}(2\overline{\Phi}'U_0,\tilde{a}_{+,\tilde{x}})+e^{-2i\tau\psi(\tilde{x})}(2\overline{\Phi}'U_0,\tilde{a}_{-,\tilde{x}}))d\sigma\\ &\quad +o(\frac{1}{\tau}).\end{aligned}$$

Integrating by parts, we obtain that there exist constants $\kappa_{2,j}$ independent of τ such that

(5.13)

$$\begin{aligned}&\int_\Omega (2\mathcal{A}\partial_z(U_{0,\tau}e^{\tau\Phi})+2\mathcal{B}\partial_{\overline{z}}(U_{0,\tau}e^{\tau\Phi}),\tilde{V}_{0,\tau}e^{-\tau\Phi})dx\\ &= (2\mathcal{A}(\partial_zU_{0,\tau}+\tau\Phi'U_{0,\tau})+2\mathcal{B}\partial_{\overline{z}}U_{0,\tau},\tilde{V}_{0,\tau})_{L^2(\Omega)}\\ &= \tau\kappa_{2,1}+\kappa_{1,0}+\frac{\kappa_{2,-1}}{\tau}\\ &\quad +\frac{1}{\tau}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}(2\mathcal{A}a_{+,\tilde{x}}\Phi',\tilde{V}_0)_{L^2(\Omega)}+e^{-2i\tau\psi(\tilde{x})}(2\mathcal{A}a_{-,\tilde{x}}\Phi',\tilde{V}_0)_{L^2(\Omega)})\\ &\quad +\frac{1}{\tau}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}(2\mathcal{A}\Phi'\tilde{U}_0,\tilde{b}_{+,\tilde{x}})_{L^2(\Omega)}+e^{-2i\tau\psi(\tilde{x})}(2\mathcal{A}\Phi'\tilde{U}_0,\tilde{b}_{-,\tilde{x}})_{L^2(\Omega)})+o(\frac{1}{\tau}).\end{aligned}$$

Since by (4.6), (4.21), (4.41) and (4.49) we have

$$-(2\mathcal{A}a_{\pm,\tilde{x}}\Phi',\tilde{V}_0)=4\partial_{\overline{z}}(a_{\pm,\tilde{x}}\Phi',\tilde{V}_0)\ \text{and}\ -(2\mathcal{A}\Phi'\tilde{U}_0,\tilde{b}_{\pm,\tilde{x}})=4\partial_{\overline{z}}(\Phi'\tilde{U}_0,\tilde{b}_{\pm,\tilde{x}})\ \text{in}\ \Omega$$

for any $\tilde{x}$ from $\mathcal{H}$, we obtain from (5.13)

(5.14)

$$\begin{aligned}\mathcal{M}_3 &:= \int_\Omega (2\mathcal{A}\partial_z(U_{0,\tau}e^{\tau\Phi})+2\mathcal{B}\partial_{\overline{z}}(U_{0,\tau}e^{\tau\Phi}),\tilde{V}_{0,\tau}e^{-\tau\Phi})dx\\ &= \tau\kappa_{2,1}+\kappa_{1,0}+\frac{\kappa_{2,-1}}{\tau}\\ &\quad -\int_{\partial\Omega}(\nu_1+i\nu_2)\frac{1}{\tau}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}(2a_{+,\tilde{x}}\Phi',\tilde{V}_0)+e^{-2i\tau\psi(\tilde{x})}(2a_{-,\tilde{x}}\Phi',\tilde{V}_0))d\sigma\\ &\quad -\int_{\partial\Omega}(\nu_1+i\nu_2)\frac{1}{\tau}\sum_{\tilde{x}\in\mathcal{H}}(e^{2i\tau\psi(\tilde{x})}(2\Phi'\tilde{U}_0,\tilde{b}_{+,\tilde{x}})+e^{-2i\tau\psi(\tilde{x})}(2\Phi'\tilde{U}_0,\tilde{b}_{-,\tilde{x}}))d\sigma\\ &\quad +o(\frac{1}{\tau}).\end{aligned}$$

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Integrating by parts, using (4.6) and Proposition 5.1, we see that there exist some constants $\kappa_{3,j}$ independent of τ such that

$$
\begin{aligned}
\mathcal{M}_4 &:= \int_\Omega (2\mathcal{A}\partial_z(\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}) + 2\mathcal{B}\partial_{\overline{z}}(\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}), \tilde{V}_{0,\tau}e^{-\tau\Phi})dx \\
&= \int_\Omega ((2\mathcal{A}\partial_z\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}, \tilde{V}_{0,\tau}e^{-\tau\Phi}) - (2\partial_{\overline{z}}\mathcal{B}\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}, \tilde{V}_{0,\tau}e^{-\tau\Phi}) \\
&\quad - (2\mathcal{B}\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}, \partial_{\overline{z}}\tilde{V}_{0,\tau}e^{-\tau\Phi}))dx \\
&\quad + \int_{\partial\Omega} (\nu_1 + i\nu_2)(\mathcal{B}\tilde{U}_{0,\tau}e^{\tau\overline{\Phi}}, \tilde{V}_{0,\tau}e^{-\tau\Phi})d\sigma \qquad (5.15)\\
&= \sum_{\tilde{x}\in\mathcal{H}} e^{-2i\tau\psi(\tilde{x})}\mathfrak{F}_{-\tau,\tilde{x}}((2\mathcal{A}\partial_z\tilde{U}_0, \tilde{V}_0) - (2\partial_{\overline{z}}\mathcal{B}\tilde{U}_0, \tilde{V}_0) - (2\mathcal{B}\tilde{U}_0, \partial_{\overline{z}}\tilde{V}_0)) \\
&\quad + \mathfrak{I}_{-\tau}((2\mathcal{A}\partial_z\tilde{U}_{0,\tau}, \tilde{V}_{0,\tau}) - (2\partial_{\overline{z}}\mathcal{B}\tilde{U}_{0,\tau}, \tilde{V}_{0,\tau}) - (2\mathcal{B}\tilde{U}_{0,\tau}, \partial_{\overline{z}}\tilde{V}_{0,\tau})) \\
&\quad + \int_{\tilde{\Gamma}} (\nu_1 + i\nu_2)(\mathcal{B}\tilde{U}_0e^{\tau\overline{\Phi}}, \tilde{V}_0e^{-\tau\Phi})d\sigma + \kappa_{3,1} + \frac{\kappa_{3,-1}}{\tau} + o(\frac{1}{\tau}).
\end{aligned}
$$

Integrating by parts and using Proposition 5.1, we obtain

(5.16)

$$
\begin{aligned}
\mathcal{M}_5 &:= \int_\Omega (2\mathcal{A}\partial_z(U_1e^{\tau\Phi}) + 2\mathcal{B}\partial_{\overline{z}}(U_1e^{\tau\Phi}), V_{0,\tau}e^{-\tau\overline{\Phi}})dx \\
&= \int_\Omega (\mathcal{A}(-B_1U_1 - e_1q_1)e^{\tau\Phi} - 2\partial_{\overline{z}}\mathcal{B}(U_1e^{\tau\Phi}), V_{0,\tau}e^{-\tau\overline{\Phi}})dx + o(\frac{1}{\tau}) \\
&\quad + \int_{\partial\Omega} (\nu_1 + i\nu_2)(\mathcal{B}U_1, V_{0,\tau})e^{\tau(\Phi-\overline{\Phi})}d\sigma - (2\mathcal{B}U_1, \partial_{\overline{z}}(V_{0,\tau}e^{\tau(\Phi-\overline{\Phi})}))_{L^2(\Omega)} \\
&= \int_\Omega (\mathcal{A}(B_1T_{B_1}(e^{\tau(\Phi-\overline{\Phi})}e_1q_1) - e_1q_1)e^{\tau(\Phi-\overline{\Phi})}, V_{0,\tau}) \\
&\quad + 2\partial_z\mathcal{B}(T_{B_1}(e^{\tau(\Phi-\overline{\Phi})}e_1q_1)), V_{0,\tau})dx \\
&\quad + (\mathcal{B}T_{B_1}(e^{\tau(\Phi-\overline{\Phi})}e_1q_1), A_2^*V_{0,\tau} - 2\tau\overline{\Phi}'V_{0,\tau})_{L^2(\Omega)} \\
&\quad + \int_{\partial\Omega} (\nu_1 + i\nu_2)(\mathcal{B}U_1, V_{0,\tau})e^{\tau(\Phi-\overline{\Phi})}d\sigma + o(\frac{1}{\tau}) \\
&= \sum_{\tilde{x}\in\mathcal{H}} e^{2i\tau\psi(\tilde{x})}\mathfrak{F}_{\tau,\tilde{x}}(q_1, T_{B_1}^*(B_1^*\mathcal{A}^*V_0) - \mathcal{A}^*V_0 \\
&\quad + 2T_{B_1}^*(\partial_z\mathcal{B}^*V_0) + T_{B_1}^*(\mathcal{B}^*(A_2^*V_0 - 2\tau\overline{\Phi}'V_0))) \\
&\quad + \int_{\partial\Omega} (\nu_1 + i\nu_2)(\mathcal{B}U_1, V_{0,\tau})e^{\tau(\Phi-\overline{\Phi})}d\sigma + o(\frac{1}{\tau}).
\end{aligned}
$$

After integration by parts, we have

$$
\begin{aligned}
\mathcal{M}_6 &:= \int_\Omega (2\mathcal{A}\partial_z(U_1e^{\tau\Phi}) + 2\mathcal{B}\partial_{\overline{z}}(U_1e^{\tau\Phi}), \tilde{V}_{0,\tau}e^{-\tau\Phi})dx \\
&= \int_\Omega (\mathcal{A}(-B_1U_1 - e_1q_1) - 2\partial_{\overline{z}}\mathcal{B}U_1, \tilde{V}_{0,\tau})dx + o(\frac{1}{\tau}) \\
&\quad + (2\mathcal{B}U_1, \partial_{\overline{z}}\tilde{V}_0)_{L^2(\Omega)} + \int_{\partial\Omega} (\nu_1 + i\nu_2)(\mathcal{B}U_1, \tilde{V}_{0,\tau})d\sigma.
\end{aligned}
$$

Using (5.8), (4.19), (4.20) and Proposition 8 of [**7**], we obtain that

$$\mathcal{M}_6 = -\int_\Omega (\mathcal{A}q_1, \tilde{V}_{0,\tau})dx + o(\frac{1}{\tau^2}) \quad \text{as} \quad \tau \to +\infty. \tag{5.17}$$

Integrating by parts and using Proposition, 5.1 we have

$$\begin{aligned}
\mathcal{M}_7 &:= \int_\Omega (2\mathcal{A}\partial_z(U_{0,\tau}e^{\tau\Phi}) + 2\mathcal{B}\partial_{\overline{z}}(U_{0,\tau}e^{\tau\Phi}), V_1 e^{-\tau\overline{\Phi}})dx \\
&= 2\int_\Omega (\mathcal{A}(\partial_z U_{0,\tau} + \tau\Phi' U_{0,\tau})e^{\tau\Phi} + \mathcal{B}\partial_{\overline{z}}U_{0,\tau}e^{\tau\Phi}, V_1 e^{-\tau\overline{\Phi}})dx \\
&= -2\int_\Omega (P^*_{-A_2^*}(\mathcal{A}(\partial_z U_0 + \tau\Phi' U_0) + \mathcal{B}\partial_{\overline{z}}U_{0,\tau}), e_1 q_4 e^{\tau(\Phi-\overline{\Phi})})dx + o(\frac{1}{\tau}) \\
&= -2\sum_{\tilde{x}\in\mathcal{H}} e^{2i\tau\psi(\tilde{x})}\mathfrak{F}_{\tau,\tilde{x}}(P^*_{-A_2^*}(\mathcal{A}(\partial_z U_0 + \tau\Phi' U_0) + \mathcal{B}\partial_{\overline{z}}U_0), q_4) \\
&\quad + o(\frac{1}{\tau}) \quad \text{as} \quad \tau \to +\infty.
\end{aligned} \tag{5.18}$$

Integrating by parts and using Proposition 4.8 and Proposition 8 of [**7**], we have

$$\begin{aligned}
\mathcal{M}_8 &:= \int_\Omega (2\mathcal{A}\partial_z(U_{0,\tau}e^{\tau\Phi}) + 2\mathcal{B}\partial_{\overline{z}}(U_{0,\tau}e^{\tau\Phi}), \tilde{V}_1 e^{-\tau\Phi})dx \\
&= \int_\Omega ((-2\partial_z\mathcal{A}U_0 + \mathcal{B}\partial_{\overline{z}}U_0, \tilde{V}_1) - (\mathcal{A}U_0, -B_2^*\tilde{V}_1 - e_1 q_3))dx + o(\frac{1}{\tau}) \\
&\quad + \int_{\partial\Omega} (\nu_1 - i\nu_2)(\mathcal{A}U_0, \tilde{V}_1)d\sigma = -\int_\Omega (\mathcal{A}U_{0,\tau}, q_3)dx + o(\frac{1}{\tau}) \quad \text{as} \quad \tau \to +\infty
\end{aligned} \tag{5.19}$$

and

$$\begin{aligned}
\mathcal{M}_9 &:= \int_\Omega (2\mathcal{A}\partial_z(\tilde{U}_1 e^{\tau\overline{\Phi}}) + 2\mathcal{B}\partial_{\overline{z}}(\tilde{U}_1 e^{\tau\overline{\Phi}}), V_{0,\tau}e^{-\tau\overline{\Phi}})dx \\
&= \int_\Omega [(\tilde{U}_1, -\partial_z(2\mathcal{A}^* V_{0,\tau})) + (\mathcal{B}(-A_1\tilde{U}_1 - e_1 q_2), V_{0,\tau})]dx + o(\frac{1}{\tau}) \\
&\quad + \int_{\partial\Omega} (\nu_1 - i\nu_2)(\mathcal{A}\tilde{U}_1, V_0)d\sigma = -\int_\Omega (\mathcal{B}q_2, V_{0,\tau})dx + o(\frac{1}{\tau}) \quad \text{as} \quad \tau \to +\infty.
\end{aligned} \tag{5.20}$$

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Integrating by parts and using Proposition 5.1, we obtain

(5.21)
$$\begin{aligned}
\mathcal{M}_{10} &:= \int_\Omega (2\mathcal{A}\partial_z(\tilde{U}_1 e^{\tau\overline{\Phi}}) + 2\mathcal{B}\partial_{\overline{z}}(\tilde{U}_1 e^{\tau\overline{\Phi}}), \tilde{V}_{0,\tau} e^{-\tau\Phi})dx \\
&= \int_\Omega ((\tilde{U}_1, -\partial_z(2\mathcal{A}^*\tilde{V}_{0,\tau}) + \tau\Phi' 2\mathcal{A}^*\tilde{V}_{0,\tau}) + (\mathcal{B}(-A_1\tilde{U}_1 - e_1 q_2), \tilde{V}_{0,\tau}) e^{\tau(\overline{\Phi}-\Phi)})dx \\
&\quad + o(\frac{1}{\tau}) + \int_{\partial\Omega} (\nu_1 - i\nu_2)(\mathcal{A}\tilde{U}_1, \tilde{V}_{0,\tau}) e^{\tau(\overline{\Phi}-\Phi)} d\sigma \\
&= \int_\Omega (e_1 q_2, P_{A_1}^*(2\partial_z(\mathcal{A}^*\tilde{V}_{0,\tau}) - 2\tau\Phi'\mathcal{A}^*\tilde{V}_0) - \mathcal{B}^*\tilde{V}_0 - P_{A_1}^*(A_1^*\mathcal{B}^*\tilde{V}_0))) e^{\tau(\overline{\Phi}-\Phi)} dx \\
&\quad + \int_{\partial\Omega} (\nu_1 - i\nu_2)(\mathcal{A}\tilde{U}_1, \tilde{V}_0) e^{\tau(\overline{\Phi}-\Phi)} d\sigma + o(\frac{1}{\tau}) \\
&= \sum_{\tilde{x}\in\mathcal{H}} e^{-2i\tau\psi(\tilde{x})} \mathfrak{F}_{-\tau,\tilde{x}}(q_2, P_{A_1}^*(2\partial_z(\mathcal{A}^*\tilde{V}_0) - \tau\Phi' 2\mathcal{A}^*\tilde{V}_0) \\
&\quad - \mathcal{B}^*\tilde{V}_0 + P_{A_1}^*(A_1^*\mathcal{B}^*\tilde{V}_0)) + o(\frac{1}{\tau}) \quad \text{as} \quad \tau \to +\infty.
\end{aligned}$$

By (4.14) and Proposition 5.1, we obtain

(5.22)
$$\begin{aligned}
\mathcal{M}_{11} &:= \int_\Omega (2\mathcal{A}\partial_z(\tilde{U}_{0,\tau} e^{\tau\overline{\Phi}}) + 2\mathcal{B}\partial_{\overline{z}}(\tilde{U}_{0,\tau} e^{\tau\overline{\Phi}}), \tilde{V}_1 e^{-\tau\Phi})dx \\
&= \int_\Omega ((2\mathcal{A}\partial_z\tilde{U}_{0,\tau} + 2\mathcal{B}(\partial_{\overline{z}}\tilde{U}_{0,\tau} + \tau\overline{\Phi}'\tilde{U}_{0,\tau}), \tilde{V}_1) e^{\tau(\overline{\Phi}-\Phi)} dx \\
&= -\int_\Omega (e_1 q_3, T_{-B_2^*}^*(2\mathcal{A}\partial_z\tilde{U}_{0,\tau} + 2\mathcal{B}(\partial_{\overline{z}}\tilde{U}_{0,\tau} + \tau\overline{\Phi}'\tilde{U}_{0,\tau})) e^{\tau(\overline{\Phi}-\Phi)} dx + o(\frac{1}{\tau}) \\
&= -\sum_{\tilde{x}\in\mathcal{H}} e^{-2i\tau\psi(\tilde{x})} \mathfrak{F}_{-\tau,\tilde{x}}(q_3, T_{-B_2^*}^*(2\mathcal{A}\partial_z\tilde{U}_0 + 2\mathcal{B}(\partial_{\overline{z}}\tilde{U}_0 + \tau\overline{\Phi}'\tilde{U}_0))) \\
&\quad + o(\frac{1}{\tau}) \quad \text{as} \quad \tau \to +\infty.
\end{aligned}$$

By Proposition 5.1, there exist constants $\kappa_{4,j}$ independent of τ such that

$$\begin{aligned}
\mathcal{M}_{12} &:= \int_\Omega (\mathcal{Q}(U_{0,\tau} e^{\tau\overline{\Phi}} + \tilde{U}_{0,\tau} e^{\tau\Phi}), V_{0,\tau} e^{-\tau\overline{\Phi}} + \tilde{V}_{0,\tau} e^{-\tau\Phi})dx \\
&= \kappa_{4,0} + \kappa_{4,-1}/\tau + \sum_{\tilde{x}\in\mathcal{H}} \frac{\pi}{2\tau|det\,\psi''(\tilde{x})|^{\frac{1}{2}}} ((\mathcal{Q}U_0, V_0)(\tilde{x}) e^{2i\tau\psi(\tilde{x})} \\
&\quad + (\mathcal{Q}\tilde{U}_0, \tilde{V}_0)(\tilde{x}) e^{-2i\tau\psi(\tilde{x})}) + o(\frac{1}{\tau}) \quad \text{as} \quad \tau \to +\infty.
\end{aligned} \tag{5.23}$$

Since $\mathcal{J}_\tau = \sum_{k=1}^{12} \mathcal{M}_k$ the proof of Proposition 5.2 is complete. ■

By Proposition 5.2, we obtain

$$\int_{\partial\Omega} ((\nu_1 + i\nu_2)\Phi'(\tilde{U}_0, V_0) + (\nu_1 - i\nu_2)\overline{\Phi}'(U_0, \tilde{V}_0))d\sigma = 0. \tag{5.24}$$

Similarly to Section 3 in [**10**], we can prove the following proposition.

PROPOSITION 5.3. *There exist a holomorphic function* $\Theta \in W_2^{\frac{1}{2}}(\Omega)$ *and an antiholomorphic function* $\widetilde{\Theta} \in W_2^{\frac{1}{2}}(\Omega)$ *such that*

$$\widetilde{\Theta}|_{\widetilde{\Gamma}} = \mathcal{C}_2^* \mathcal{C}_1, \quad \Theta|_{\widetilde{\Gamma}} = \mathcal{P}_2^* \mathcal{P}_1 \tag{5.25}$$

and

$$\Theta = \tilde{\Theta} \quad on \quad \Gamma_0. \tag{5.26}$$

Let $\tilde{\gamma}$ be a curve which does not intersect itself and passes through the point $\hat{x}$ and couple points x_1, x_2 from $\tilde{\Gamma}$ such that the set $\tilde{\gamma} \cap \partial\Omega \setminus \{x_1, x_2\}$ is empty. Denote by Ω_1 the domain bounded by $\tilde{\gamma}$ and the part of $\partial\Omega$ located between the points x_1 and x_2. Repeating the arguments in [**10**], we construct a smooth invertible matrix $\mathbf{Q}$ such that for the operator $\mathbf{Q}^{-1} L_1(x,D)\mathbf{Q}$ and the operator $L_1(x,D)$, the corresponding Dirichlet-to-Neumann maps are the same, the equality (5.25) holds on $\partial\Omega$ instead of $\tilde{\Gamma}$ and $\mathbf{Q}$ is the identity matrix in Ω_1. From now on we work with the operator $\mathbf{Q}^{-1} L_1(x,D)\mathbf{Q}$ instead of $L_1(x,D)$.

In view of Proposition 5.2, repeating the arguments of the proof of Proposition 4.5 in [**10**], we obtain

PROPOSITION 5.4. *Under the assumptions of Proposition* 5.2*, we have*

$$T^*_{B_1}(\mathcal{B}^* \overline{\Phi}' V_0) = P^*_{-A_2^*}(\mathcal{A}\Phi' V_0) = P^*_{A_1}(\mathcal{B}\Phi' \tilde{V}_0) = T^*_{-B_2^*}(\mathcal{A}^* \overline{\Phi}' \tilde{U}_0) = 0 \quad on \quad \tilde{\Gamma} \tag{5.27}$$

and

$$T^*_{B_1}(\mathcal{B}^* V_0) = P^*_{-A_2^*}(\mathcal{A} V_0) = P^*_{A_1}(\mathcal{B}\tilde{V}_0) = T^*_{-B_2^*}(\mathcal{A}^* \tilde{U}_0) = 0 \quad on \quad \tilde{\Gamma}. \tag{5.28}$$

Using Proposition 5.4, we prove

PROPOSITION 5.5. *Under the assumptions of Proposition* 5.2*, we have*

$$P^*_{-A_2^*}(\mathcal{A}U_0\Phi') = \Phi' P^*_{-A_2^*}(\mathcal{A}U_0), \quad T_{B_1}(\mathcal{B}^* \overline{\Phi}' V_0) = \overline{\Phi}' T_{B_1}(\mathcal{B}^* V_0) \tag{5.29}$$

and

$$P^*_{A_1^*}(\mathcal{A}^* \tilde{V}_0 \Phi') = \Phi' P^*_{A_1^*}(\mathcal{A}^* \tilde{V}_0), \quad T^*_{-B_2^*}(\mathcal{B}\overline{\Phi}' \tilde{U}_0) = \overline{\Phi}' T^*_{-B_2^*}(\mathcal{B}^* \tilde{U}_0). \tag{5.30}$$

Proof. We prove the first equality in (5.29). The proofs of the remaining three equalities are the same. By (5.27) and (5.28), we have

$$P^*_{-A_2^*}(\mathcal{A}U_0\Phi') = \Phi' P^*_{-A_2^*}(\mathcal{A}U_0) = 0 \quad \text{on } \tilde{\Gamma}.$$

We set $r_1 = P^*_{-A_2^*}(\mathcal{A}U_0\Phi')$ and $r_2 = \Phi' P^*_{-A_2^*}(\mathcal{A}U_0)$. Then the functions r_j satisfy

$$-2\partial_{\overline{z}} r_j - A_2^* r_j = \mathcal{A}U_0\Phi' \quad \text{in } \Omega, \quad r_j|_{\tilde{\Gamma}} = 0 \quad \forall j \in \{1,2\}.$$

By the uniqueness of the Cauchy problem for the operator $\partial_{\overline{z}}$, we have that $r_1 = r_2$. The proof of Proposition 5.5 is complete. ■

We use Proposition 5.5 to simplify the formula (5.2).

PROPOSITION 5.6. *Under the conditions of Proposition* 5.2*, we have*

$$\begin{aligned} &-(2\partial_z \mathcal{A}U_0, V_0)(\tilde{x}) - (2\mathcal{A}U_0, \partial_z V_0)(\tilde{x}) + (2\mathcal{B}\partial_{\overline{z}} U_0, V_0)(\tilde{x}) \\ &-((Q_1(1)U_0, T^*_{B_1}(\mathcal{B}^* V_0)) + (Q_2(2)V_0, P^*_{-A_2^*}(\mathcal{A}U_0)))(\tilde{x}) \\ &+(\mathcal{Q}U_0, V_0)(\tilde{x}) + I_{+,\Phi}(\tilde{x}) = 0 \quad in \ \Omega, \end{aligned} \tag{5.31}$$

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where the function Φ *satisfies (*4.2*) and*

$$Im\,\Phi(\widetilde{x}) \notin \{Im\,\Phi(x);\, x \in \mathcal{H} \setminus \{\widetilde{x}\}\}. \tag{5.32}$$

Proof. By Proposition 5.2, equality (5.2) holds true. Thanks to (5.32) and Proposition 5.4, we can write it as

$$(J_+ + K_+)(\tilde{x}) + I_{+,\Phi}(\tilde{x}) = 0. \tag{5.33}$$

By Propositions 5.1 and 5.5, we obtain

$$\begin{aligned}
&\mathfrak{F}_{\tau,\tilde{x}}(q_1, T^*_{B_1} B_1^* \mathcal{A}^* V_0 - \mathcal{A}^* V_0 + 2T^*_{B_1}\partial_z \mathcal{B}^* V_0 + T^*_{B_1}(\mathcal{B}^*(A_2^* V_0 - 2\tau\overline{\Phi}' V_0))) \\
&\quad = -\mathfrak{F}_{\tau,\tilde{x}}(q_1, T^*_{B_1}(\mathcal{B}^* 2\tau\overline{\Phi}' V_0)) + o(\frac{1}{\tau}) \\
&\quad = -\mathfrak{F}_{\tau,\tilde{x}}(q_1, 2\tau\overline{\Phi}' T^*_{B_1}(\mathcal{B}^* V_0)) + o(\frac{1}{\tau}) \\
&\quad = -\frac{\pi}{2\tau|det\,\psi''(\tilde{x})|^{\frac{1}{2}}}(2\partial_{\overline{z}} q_1, T^*_{B_1}(\mathcal{B}^* V_0))(\tilde{x}) + o(\frac{1}{\tau}) \\
&\quad = -\frac{\pi}{2\tau|det\,\psi''(\tilde{x})|^{\frac{1}{2}}}(Q_1(1)U_0, T^*_{B_1}(\mathcal{B}^* V_0))(\tilde{x}) + o(\frac{1}{\tau})
\end{aligned} \tag{5.34}$$

and

$$\begin{aligned}
&-2\mathfrak{F}_{\tau,\tilde{x}}(P^*_{-A_2^*}(\mathcal{A}(\partial_z U_0 + \tau\Phi' U_0)) + \mathcal{B}\partial_{\overline{z}} U_{0,\tau}, q_4) \\
&\quad = -2\mathfrak{F}_{\tau}(P^*_{-A_2^*}(\mathcal{A}\tau\Phi' U_0), q_4) + o(\frac{1}{\tau}) \\
&\quad = -2\mathfrak{F}_{\tau,\tilde{x}}(\tau\Phi' P^*_{-A_2^*}(\mathcal{A}U_0), q_4) + o(\frac{1}{\tau}) \\
&\quad = \frac{\pi}{2\tau|det\,\psi''(\tilde{x})|^{\frac{1}{2}}}(P^*_{-A_2^*}(\mathcal{A}U_0), 2\partial_z q_4)(\tilde{x}) + o(\frac{1}{\tau}) \\
&\quad = \frac{\pi}{2\tau|det\,\psi''(\tilde{x})|^{\frac{1}{2}}}(P^*_{-A_2^*}(\mathcal{A}U_0), Q_2(2)V_0)(\tilde{x}) + o(\frac{1}{\tau}).
\end{aligned} \tag{5.35}$$

Equalities (5.34) and (5.35) yield

$$K_+(\tilde{x}) = \frac{\pi}{2\tau|det\,\psi''(\tilde{x})|^{\frac{1}{2}}}(-(Q_1(1)U_0, T^*_{B_1}(\mathcal{B}^* V_0))(\tilde{x}) + (P^*_{-A_2^*}(\mathcal{A}U_0), Q_2(2)V_0)(\tilde{x})). \tag{5.36}$$

Substituting into (5.33) the right-hand side of (5.36), we obtain (5.31). The proof of the proposition is complete. ■

6. Step 5: End of the proof

Suppose that for the operators $L_{\mu_1,\gamma_1}(x,D)$ and $L_{\mu_2,\gamma_2}(x,D)$ given by (1.5) the Dirichlet-to-Neumann maps Λ_{μ_j,γ_j} given by (1.7) are the same. Then, by Proposition 2.1 the Dirichlet-to-Neumann maps for the operators $L_1(x,D)$ and $L_2(x,D)$ given by formula (2.19) are the same. Let u_1 be the complex geometric optics solution constructed by (4.39) for the operator $L_1(x,D)$. There exists a solution u_2 to the following boundary value problem:

$$L_2(x,D)u_2 = 0 \quad \text{in } \Omega, \quad \mathcal{B}(x,D)(u_1 - u_2)|_{\partial\Omega} = 0, \quad \mathcal{R}(x,D)(u_1 - u_2) = 0 \quad \text{on } \tilde{\Gamma}.$$

Setting $u = u_1 - u_2$, we have

$$L_2(x,D)u + 2\mathcal{A}\partial_z u_1 + 2\mathcal{B}\partial_{\overline{z}} u_1 + \mathcal{Q}u_1 = 0 \quad \text{in } \Omega \tag{6.1}$$

and

$$\mathcal{B}(x,D)u|_{\partial\Omega} = 0, \quad \mathcal{R}(x,D)u|_{\widetilde{\Gamma}} = 0. \tag{6.2}$$

Let v be a function given by (4.59). Taking the scalar product of (6.1) with v in $L^2(\Omega)$ and using (4.60) and (6.2), we obtain

$$0 = \mathfrak{G}(u_1, v) := \int_\Omega (2\mathcal{A}\partial_z u_1 + 2\mathcal{B}\partial_{\overline{z}} u_1 + \mathcal{Q}u_1, v)dx. \tag{6.3}$$

PROPOSITION 6.1. *Let u_1 be given by (4.39) and v be given by (4.59). Then*

$$\mathfrak{G}(u_1, v) = \int_\Omega (2\mathcal{A}\partial_z U + 2\mathcal{B}\partial_{\overline{z}} U + \mathcal{Q}U, V^*)dx + o(\frac{1}{\tau}) \quad as \quad \tau \to +\infty.$$

Here U and V are defined by (4.26) and (4.55) respectively.

Proof. Since the form $\mathfrak{G}(\cdot,\cdot)$ is bilinear in order to prove the statement of this proposition it suffices to show that

$$\mathfrak{G}(e^{\tau\varphi}\tilde{u}_{-1}, V^*) = \mathfrak{G}(e^{\tau\varphi}\tilde{u}_{-1}, e^{-\tau\varphi}v_{-1}) = \mathfrak{G}(U, e^{-\tau\varphi}v_{-1}) = o(\frac{1}{\tau}) \quad \text{as } \tau \to +\infty. \tag{6.4}$$

Obviously, by (4.38) and (4.58), we see that

$$\mathfrak{G}(e^{\tau\varphi}\tilde{u}_{-1}, e^{-\tau\varphi}v_{-1}) = o(\frac{1}{\tau}) \quad \text{as } \tau \to +\infty. \tag{6.5}$$

Let $\chi \in C_0^\infty(\Omega)$ satisfy $\chi|_{\Omega\setminus\mathcal{O}_{\frac{\varepsilon}{2}}} = 1$. By (4.38), we have

$$\begin{aligned} \mathfrak{G}(e^{\tau\varphi}\tilde{u}_{-1}, V^*) &= \mathfrak{G}(e^{\tau\varphi}\tilde{u}_{-1}, \chi V^*) + o(\frac{1}{\tau}) \\ &= \int_\Omega (2\mathcal{A}\partial_z(e^{\tau\varphi}\tilde{u}_{-1}) + 2\mathcal{B}\partial_{\overline{z}}(e^{\tau\varphi}\tilde{u}_{-1}), \chi V^*)dx + o(\frac{1}{\tau}) \\ &= \int_\Omega (2\mathcal{A}\partial_z(e^{\tau\varphi}\tilde{u}_{-1}), \chi\tilde{V}_0 e^{-\tau\overline{\Phi}}) + (2\mathcal{B}\partial_{\overline{z}}(e^{\tau\varphi}\tilde{u}_{-1}), \chi V_0 e^{-\tau\Phi})dx + o(\frac{1}{\tau}). \end{aligned} \tag{6.6}$$

Let functions w_4, w_5 solve the equations $(-\partial_{\overline{z}} + B_1^*)w_4 = 2\mathcal{A}^* V_0$ and $(-\partial_z + A_1^*)w_5 = 2\mathcal{B}^*\tilde{V}_0$.

Taking the scalar product of equation (4.37) and the function $\chi(w_5 e^{\tau\Phi} + w_4 e^{\tau\overline{\Phi}})$, after integration by parts we obtain

$$\begin{aligned} \int_\Omega ((2\partial_z(e^{\tau\varphi}\tilde{u}_{-1}) + A_1(e^{\tau\varphi}\tilde{u}_{-1}), 2\mathcal{A}^*\widetilde{V}_0 e^{-\tau\overline{\Phi}}) \\ +(2\partial_{\overline{z}}(e^{\tau\varphi}\tilde{u}_{-1}) + B_1(e^{\tau\varphi}\tilde{u}_{-1}), 2\mathcal{B}^*\tilde{V}_0 e^{-\tau\Phi}))dx = o(\frac{1}{\tau}). \end{aligned} \tag{6.7}$$

By (6.6) and (6.7), we obtain the first equality in (6.4). The proof of the second equality in (6.4) is the same and involves the estimate (4.58). ■

Thanks to Proposition 6.1, the statements of Propositions 5.2–5.5 hold true.

PROPOSITION 6.2. *Let the sequence of functions Φ_ϵ be given by Proposition 4.1. For the functions $I_{\pm,\Phi_\epsilon}$ given by (5.5) and (5.6), we have*

$$I_{\pm,\Phi_\epsilon}(\tilde{x}_\epsilon) \equiv 0 \quad x_\epsilon \in \mathcal{H}. \tag{6.8}$$

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Proof. We prove this statement for the function I_{+,Φ_ϵ}. The proof for the function I_{-,Φ_ϵ} is the same. We choose $\widetilde{a}_{\pm,\tilde{x}_\epsilon}, \widetilde{b}_{\pm,\tilde{x}_\epsilon}$ in the form

$$(\widetilde{a}_{\pm,\tilde{x}_\epsilon}, \widetilde{b}_{\pm,\tilde{x}_\epsilon}) = (\mathcal{C}_2(x)\widetilde{\mathbf{a}}_{\pm,\tilde{x}_\epsilon}(\overline{z}), \mathcal{P}_2(x)\widetilde{\mathbf{b}}_{\pm,\tilde{x}_\epsilon}(z)), \tag{6.9}$$

where $\mathbf{a}_{\pm,\tilde{x}}(\overline{z})$ is some antiholomorphic function and $\mathbf{b}_{\pm,\tilde{x}}(z)$ is some holomorphic function. Similarly choose the functions $a_{\pm,\tilde{x}_\epsilon}, b_{\pm,\tilde{x}_\epsilon}$ in the form

$$(a_{\pm,\tilde{x}_\epsilon}, b_{\pm,\tilde{x}_\epsilon}) = (\mathcal{P}_1(x)\mathbf{a}_{\pm,\tilde{x}_\epsilon}(z), \mathcal{C}_1(x)\mathbf{b}_{\pm,\tilde{x}_\epsilon}(\overline{z})). \tag{6.10}$$

The pairs $(U_0, \tilde{U}_0)$ and $(V_0, \tilde{V}_0)$ are constructed in the following way:

$$U_0 = \mathcal{P}_1\mathbf{a}, \quad \tilde{U}_0 = \mathcal{C}_1\overline{\mathbf{a}}, \quad V_0 = \mathcal{C}_2\overline{\mathbf{b}}, \quad \tilde{V}_0 = \mathcal{P}_2\mathbf{b}, \tag{6.11}$$

where $\mathbf{a}(z) = (a_1(z), \dots, a_N(z)) \in C^{5+\alpha}(\overline{\Omega})$ is a holomorphic vector function such that $\operatorname{Re}\mathbf{a}|_{\Gamma_0} = 0$ and $\mathbf{b}(z) = (b_1(z), \dots, b_N(z)) \in C^{5+\alpha}(\overline{\Omega})$ is a holomorphic vector function such that $\operatorname{Im}\mathbf{b}|_{\Gamma_0} = 0$. Then

$$\begin{aligned} I_{+,\Phi_\epsilon}(\tilde{x}) = -\int_{\partial\Omega} \Big\{ &(\nu_1 - i\nu_2)((2\mathcal{C}_1(x)\mathbf{b}_{\pm,\tilde{x}}\overline{\Phi}'_\epsilon, \mathcal{C}_2\overline{\mathbf{b}}) + (2\overline{\Phi}'_\epsilon\mathcal{C}_1\overline{\mathbf{a}}, \mathcal{C}_2(x)\widetilde{\mathbf{a}}_{\pm,\tilde{x}_\epsilon})) \\ &+(\nu_1 + i\nu_2)((2\mathcal{P}_1(x)\mathbf{a}_{\pm,\tilde{x}}\Phi'_\epsilon, \mathcal{P}_2\mathbf{b}) + (2\Phi'_\epsilon\mathcal{P}_1\mathbf{a}, \mathcal{P}_2(x)\widetilde{\mathbf{b}}_{\pm,\tilde{x}}))\Big\}\, d\sigma = \\ -\int_{\partial\Omega} \Big\{ &(\nu_1 - i\nu_2)((2\mathcal{C}_2^*\mathcal{C}_1(x)\mathbf{b}_{\pm,\tilde{x}_\epsilon}\overline{\Phi}'_\epsilon, \overline{\mathbf{b}}) + (2\overline{\Phi}'_\epsilon\mathcal{C}_2^*\mathcal{C}_1\overline{\mathbf{a}}, \widetilde{\mathbf{a}}_{\pm,\tilde{x}_\epsilon})) \\ &+(\nu_1 + i\nu_2)((2\mathcal{P}_2^*\mathcal{P}_1(x)\mathbf{a}_{\pm,\tilde{x}}\Phi'_\epsilon, \mathbf{b}) + (2\Phi'_\epsilon\mathcal{P}_2^*\mathcal{P}_1\mathbf{a}, \widetilde{\mathbf{b}}_{\pm,\tilde{x}_\epsilon}))\Big\}\, d\sigma. \end{aligned}$$

Thanks to the gauge transformation, there exist a holomorphic function Θ in Ω and an antiholomorphic function $\tilde{\Theta}$ in Ω such that

$$\widetilde{\Theta}|_{\partial\Omega} = \mathcal{C}_2^*\mathcal{C}_1, \quad \Theta|_{\partial\Omega} = \mathcal{P}_2^*\mathcal{P}_1. \tag{6.12}$$

Hence

$$\begin{aligned} I_{+,\Phi_\epsilon}(\tilde{x}) = -\int_{\partial\Omega} \Big\{ &(\nu_1 - i\nu_2)((2\widetilde{\Theta}\mathbf{b}_{\pm,\tilde{x}_\epsilon}\overline{\Phi}'_\epsilon, \overline{\mathbf{b}}) + (2\overline{\Phi}'_\epsilon\widetilde{\Theta}\overline{\mathbf{a}}, \widetilde{\mathbf{a}}_{\pm,\tilde{x}_\epsilon})) \\ &+(\nu_1 + i\nu_2)((2\Theta\mathbf{a}_{\pm,\tilde{x}}\Phi'_\epsilon, \mathbf{b}) + (2\Phi'_\epsilon\Theta\mathbf{a}, \widetilde{\mathbf{b}}_{\pm,\tilde{x}_\epsilon}))\Big\}\, d\sigma = 0. \end{aligned}$$

This implies (6.8). ■

Since for any x from Ω, there exists a sequence of x_ϵ converging to x by (4.4), using (6.8), we rewrite the equation (5.31) as

$$\begin{aligned} &-(2\partial_z\mathcal{A}U_0, V_0) - (2\mathcal{A}U_0, \partial_z V_0) + (2\mathcal{B}\partial_{\overline{z}}U_0, V_0) \\ &-((Q_1(1)U_0, T^*_{B_1}(\mathcal{B}^*V_0)) + (Q_2(2)V_0, P^*_{-A_2^*}(\mathcal{A}U_0))) \\ &\qquad +(\mathcal{Q}U_0, V_0) = 0 \quad \text{in } \Omega. \end{aligned} \tag{6.13}$$

By Proposition 4.2 for each point $\tilde{x}$ from Ω, we can construct functions U_0, V_0 satisfying (4.7), (4.9), (4.41) and (4.42) such that

$$U_0^{(k)}(\tilde{x}) = \vec{e}_k, \quad V_0^{(\ell)}(\tilde{x}) = \vec{e}_\ell \quad \forall k, \ell \in \{1, 2\}.$$

Then for each $\tilde{x}$ there exists positive $\delta(\tilde{x})$ such that the matrices $\{U_{0,i}^{(j)}\}$ and $\{V_{0,i}^{(j)}\}$ are invertible for any $x \in \overline{B(\tilde{x}, \delta(\tilde{x}))}$: the ball centered at $\tilde{x}$ with radius $\delta(\tilde{x})$. From

the covering of Ω by such balls, we take a finite subcovering $\overline{\Omega} \subset \cup_{k=1}^{\tilde{N}} B(x_k, \delta(x_k))$. Then from (6.13) we have the differential inequality

$$|\partial_z \mathcal{A}_{ij}| \le \mathcal{C}(x)(\sum_{k=1}^{N} |T^*_{B_1}(\mathcal{B}^* V_0(k))| + |P^*_{-A_2^*}(\mathcal{A}U_0(k))| + |\mathcal{A}| + |\mathcal{B}| + |\mathcal{Q}|) \quad \text{in } \Omega, \quad \forall i,j \in \{1,2\}, \tag{6.14}$$

where $\mathcal{C}(x)$ is continuous on $\overline{\Omega} \setminus \overline{\Gamma}_0$. We set $\rho = (\rho_1(1) - \rho_1(2), \rho_2(1) - \rho_2(2), \rho_3(1) - \rho_3(2))$, where the functions $\rho_i(j)$ are defined by (2.15) with the functions μ, σ, ϵ replaced by $\mu_j, \sigma_j, \epsilon_j$. Let the point $\hat{x}$ belong to $\operatorname{supp} \rho$. Using (2.17), we rewrite (6.14) as

$$|\Delta \rho| \le \mathcal{C}(x)(\sum_{k=1}^{N} |T^*_{B_1}(\mathcal{B}^* V_0(k))| + |P^*_{-A_2^*}(\mathcal{A}U_0(k))| + |\nabla \rho| + |\rho|) \quad \text{in } \Omega. \tag{6.15}$$

Let $\tilde{\gamma}$ be a curve which does not intersects itself and passes through the point $\hat{x}$ and couple points x_1, x_2 from $\tilde{\Gamma}$ such that the set $\tilde{\gamma} \cap \partial\Omega \setminus \{x_1, x_2\}$ is empty. Denote by Ω_1 the domain bounded by $\tilde{\gamma}$ and the part of $\partial\Omega$ located between the points x_1 and x_2. Then we set $\Omega_{1,\epsilon} = \{x;\, dist(\Omega_1, x) < \epsilon\}$. Let a function ϕ_0 satisfy

$$\nabla \phi_0(x) \ne 0 \quad \text{in } \Omega_1, \quad \partial_{\tilde{\nu}} \phi_0|_{\tilde{\gamma}} \le \alpha' < 0, \quad \phi_0|_{\tilde{\gamma}} = 0, \tag{6.16}$$

where $\tilde{\nu}$ is the outward normal vector to Ω_1 and let

$$\chi_\epsilon \in C^2(\overline{\Omega_{1,\epsilon}}), \quad \chi_\epsilon = 1 \qquad \text{in } \Omega_1,$$

and $\chi_\epsilon \equiv 0$ in some neighborhood of the curve γ. We set $\rho_\epsilon = \chi_\epsilon \rho$. From (6.15), we have

$$\begin{aligned} |\Delta \rho_\epsilon| &\le \mathcal{C}(x)(\sum_{k=1}^{N} |\chi_\epsilon T^*_{B_1}(\mathcal{B}^* V_0(k))| \\ &\quad + |\chi_\epsilon P^*_{-A_2^*}(\mathcal{A}U_0(k))| + \chi_\epsilon(|\nabla \rho| + |\rho|) + |[\chi_\epsilon, \Delta]\rho|) \qquad \text{in } \Omega_{1,\epsilon}, \\ \rho_\epsilon|_{\partial\Omega_{1,\epsilon}} &= \partial_{\tilde{\nu}} \rho_\epsilon|_{\partial\Omega_{1,\epsilon}} = 0. \end{aligned}$$

The last equality follows immediately from (1.9) and the properties of the function χ_ϵ. Set $\psi_0 = e^{\lambda \phi_0}$ with positive λ sufficiently large. Applying the Carleman estimate for Δ to the above inequality we have

$$\begin{aligned} &\int_{\Omega_{1,\epsilon}} e^{2\tau\psi_0}(\tau|\nabla \rho_\epsilon|^2 + \tau^3 |\rho_\epsilon|^2) dx \le C \int_{\Omega_{1,\epsilon}} (\sum_{k=1}^{N} |\chi_\epsilon T^*_{B_1}(\mathcal{B}^* V_0(k))|^2 \\ &+ |\chi_\epsilon P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 + \chi_\epsilon^2(|\nabla \rho| + |\rho|^2) + |[\chi_\epsilon, \Delta]\rho|^2) e^{2\tau\psi_0} dx \quad \forall \tau \ge \tau_0. \end{aligned} \tag{6.17}$$

By the Carleman estimate for the operator ∂_z, there exist positive constants C and τ_0 independent of τ such that

$$\begin{aligned} &\int_{\Omega_{1,\epsilon}} |\chi_\epsilon T^*_{B_1}(\mathcal{B}^* V_0(k))|^2 e^{2\tau\psi_0} dx \\ &\qquad \le C \int_{\Omega_{1,\epsilon}} (|[\chi_\epsilon, \partial_z] T^*_{B_1}(\mathcal{B}^* V_0(k))|^2 + |\mathcal{B}^* V_0(k)|^2) e^{2\tau\psi_0} dx \end{aligned} \tag{6.18}$$

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and

$$\begin{aligned}\int_{\Omega_{1,\epsilon}} &|\chi_\epsilon P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 e^{2\tau\psi_0}dx \\ &\leq C\int_{\Omega_{1,\epsilon}} (|[\chi_\epsilon,\partial_{\overline{z}}]P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 + |\mathcal{A}U_0(k)|^2)e^{2\tau\psi_0}dx\end{aligned} \tag{6.19}$$

for all $\tau \geq \tau_0$. Combining estimates (6.17), (6.18) and (6.19), we obtain

$$\begin{aligned}\int_{\Omega_{1,\epsilon}} e^{2\tau\psi_0}(\tau|\nabla\rho_\epsilon|^2 + \tau^3|\rho_\epsilon|^2)dx &\leq C\int_{\Omega_{1,\epsilon}} (\sum_{k=1}^N |[\chi_\epsilon,\partial_{\overline{z}}]P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 \\ +|\chi_\epsilon(\mathcal{A}U_0(k))|^2 + |[\chi_\epsilon,\partial_z]T^*_{B_1}(\mathcal{B}^*V_0(k))|^2 + |\chi_\epsilon\mathcal{B}^*V_0(k)|^2 + |[\chi_\epsilon,\Delta]\rho|^2)e^{2\tau\psi_0}dx \\ &\leq C\int_{\Omega_{1,\epsilon}} (\sum_{k=1}^N |[\chi_\epsilon,\partial_{\overline{z}}]P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 + |\nabla\rho_\epsilon|^2 + |\rho_\epsilon|^2) \\ &\quad +|[\chi_\epsilon,\partial_z]T^*_{B_1}(\mathcal{B}^*V_0(k))|^2 + |[\chi_\epsilon,\Delta]\rho|^2)e^{2\tau\psi_0}dx \quad \forall\tau\geq\tau_0.\end{aligned} \tag{6.20}$$

For all sufficiently large τ the term $\int_{\Omega_{1,\epsilon}}(|\nabla\rho_\epsilon|^2+|\rho_\epsilon|^2)e^{2\tau\psi_0}dx$ can be absorbed by the integral on the left-hand side. Moreover, thanks to the choice of the functions μ_ϵ, the supports of the coefficients of the operators $[\chi_\epsilon,\partial_z]$, $[\chi_\epsilon,\partial_{\overline{z}}]$ and $[\chi_\epsilon,\Delta]$ are located in the domain $\Omega_{1,\epsilon}\setminus\Omega_{1,\frac{\epsilon}{2}}$. Hence we can write the estimate (6.21) as

$$\begin{aligned}\int_{\Omega_{1,\epsilon}} e^{2\tau\psi_0}(\tau|\nabla\rho_\epsilon|^2 + \tau^3|\rho_\epsilon|^2)dx &\leq C\int_{\Omega_{1,\epsilon}\setminus\Omega_{1,\frac{\epsilon}{2}}} (\sum_{k=1}^N |[\chi_\epsilon,\partial_{\overline{z}}]P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 \\ &\quad +|[\chi_\epsilon,\partial_z]T^*_{B_1}(\mathcal{B}^*V_0(k))|^2 + |[\chi_\epsilon,\Delta]\rho|^2)e^{2\tau\psi_0}dx \quad \forall\tau\geq\tau_1.\end{aligned} \tag{6.21}$$

By (6.16) for all sufficiently small positive ϵ, there exists a positive constant $\alpha<1$ such that

$$\tilde{\psi}_0(x) < \alpha \quad \text{on} \quad \Omega_{1,\epsilon}\setminus\Omega_{1,\frac{\epsilon}{2}}. \tag{6.22}$$

Since $\hat{x}\in\operatorname{supp}\rho\cap\tilde{\gamma}$ and $\partial_{\tilde{\nu}}\phi_0|_{\tilde{\gamma}}\leq\alpha'<0$ with some constant α', there exists $\kappa>0$ such that

$$\kappa e^\tau \leq \int_{\Omega_{1,\epsilon}} e^{2\tau\psi_0}(\tau|\nabla\rho_\epsilon|^2+\tau^3|\rho_\epsilon|^2)dx \quad \forall\tau\geq\tau_1. \tag{6.23}$$

By (6.22) we can estimate the right-hand side of the inequality (6.21) as

$$\begin{aligned}\int_{\Omega_{1,\epsilon}\setminus\Omega_{1,\frac{\epsilon}{2}}} &(\sum_{k=1}^N |[\chi_\epsilon,\partial_{\overline{z}}]P^*_{-A_2^*}(\mathcal{A}U_0(k))|^2 \\ &+|[\chi_\epsilon,\partial_z]T^*_{B_1}(\mathcal{B}^*V_0(k))|^2 + |[\chi_\epsilon,\Delta]\rho|^2)e^{2\tau\psi_0}dx \leq Ce^{\alpha\tau} \quad \forall\tau\geq\tau_1.\end{aligned} \tag{6.24}$$

Using (6.23) and (6.24) in (6.21), we obtain

$$\kappa e^\tau \leq Ce^{\alpha\tau} \quad \forall\tau\geq\tau_1.$$

Since $\alpha<1$, we reach a contradiction. ■

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Gaussian beams on Zoll manifolds and maximally degenerate Laplacians

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Abstract. Gaussian beams exist along all closed geodesics of a Zoll surface, despite the fact that the algorithm for constructing them assumes that the closed geodesics are non-degenerate. Similarly, there exists a global Birkhoff normal for a Zoll Laplacian despite the degeneracy. We explain why both algorithms work in the Zoll case and give an exact formula for the sub-principal normal form invariant. In the case of "maximally degenerate" Zoll Laplacians, this invariant vanishes and we obtain new geometric constraints on such Zoll metrics.

1. Introduction

A *Gaussian beam* is a sequence $\{\varphi_k^\gamma\}_{k=1}^\infty$ of exact or approximate eigenfunctions of the Laplacian Δ_g of a compact Riemannian manifold (M, g) which concentrates along a stable closed geodesic γ.The simplest Gaussian beams have the approximate form $e^{iks}e^{-k|y|^2}$ where (s, y) are Fermi normal coordinates with respect to γ, with y the normal coordinates and s the arc-length coordinate along γ. Thus Gaussian beams oscillate along γ but have Gaussian decay in the orthogonal direction. More generally for each $q = 0, 1, 2 \dots$, one may define higher Gaussian beams $\{\varphi_{k,q}^\gamma\}$ which are of the form $e^{iks}U_q(ky)$ where U_q is the qth Hermite function. Gaussian beams have a long history in mathematics and physics, and we refer to J. Ralston's articles [**Ra**, **Ra2**, **Ra3**] as well as [**BB**, **W**] for the some of the results.

In all of the articles known to the author, the closed geodesic is assumed to be non-degenerate stable elliptic. That is, the eigenvalues of its linear Poincaré map P_γ (defined below) are assumed to be of unit modulus $e^{i\alpha_j}$ and the Floquet exponents $\{\alpha_j, 2\pi\}$ are assumed to be independent over $\mathbb{Q}$, in particular to satisfy $e^{i(m-n)\alpha_j} \neq 1$. The non-degeneracy condition is needed to prove existence of solutions of certain transport equations. It arises for the same reason in the homological equation that appears when one tries to put Δ_g into quantum Birkhoff normal form around γ [**G2**, **Z2**]. However, non-degeneracy is not always a necessary condition for existence of Gaussian beams or normal forms: in the case of S^2, P_γ is the identity operator and its closed geodesics are degenerate. Nevertheless it possesses Gaussian beams around all closed geodesics. They are the highest weight spherical harmonics Y_ℓ^ℓ

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of degree ℓ, which concentrate along the equator. By rotating Y_ℓ^ℓ one obtains a Gaussian beam concentrating along any closed geodesic of S^2. We refer to [**SHang**, **Z4**] for background and references.

Moreover, there exist Gaussian beams along any closed geodesic of any Zoll surface, i.e. a surface all of whose geodesics are closed [**Be**], where again $P_\gamma = I$ for all γ. Unlike the case of the standard metric on S^2, the Gaussian beams are usually not eigenfunctions of Δ_g but only *quasi-modes* or approximate eigenfunctions. However, they are actual eigenfunctions in the case of maximally degenerate Laplacians (see §1.1). One of our goals is to find the obstructions to constructing Gaussian beams which solve the eigenvalue equation to arbitrarily high order, and to analyze how they can vanish in the maximally degenerate case.

As discussed in [**Z1**, **Z2**], the construction of Gaussian beams around a closed geodesic γ is closely related to the construction of a quantum Birkhoff normal form for Δ in a tubular neighborhood around γ. There are obstructions to the construction of this normal form and apriori they might not exist in the Zoll case. But in [**G**], Guillemin constructs a *global* Birkhoff normal form for the Laplacian on a Zoll surface. Hence the microlocal normal forms also exist (and coincide with the restrictions of the global one). Parallel to Gaussian beams, one of the aims of this note is to indicate why the constructions are possible for Zoll Laplacians even though they fail completely to satisfy the non-degeneracy assumptions.

The existence of the global quantum Birkhoff normal form is due to the fact that Zoll geodesic flows are symplectically equivalent. The symplectic equivalence is due to the fact that one may define a symplectic space of geodesics $G(S^2, g)$ of a Zoll surface (S^2, g). To define $G(S^2, g)$ we note that the geodesic flow of a Zoll surface (S^2, g) defines a free S^1 action on the unit cotangent bundle $S_g^* S^2$ for the metric g [**GrGr**]. The space of geodesics is defined as the orbit space,

$$G(S^2, g) := S_g^* S^2 / S^1. \tag{1}$$

It is naturally a symplectic manifold [**W**, **Be**]. Indeed, tangent vectors to geodesics are orthogonal Jacobi fields, and the symplectic form is defined by the Wronskian (see (10) of §2). By the Moser method, one may construct a symplectic diffeomorphism from $G(S^2, g)$ to the standard space $G(S^2, g_0)$ of geodesics. It lifts to a contact transformation $\chi : S_g^* S^2 \to S_{g_0}^* S^2$ of the unit cosphere bundles intertwining the geodesic flows. The symplectic map χ may be quantized to give a unitary Fourier integral operator $U = U_\chi$ which conjugates the Laplacians modulo a remainder of order zero, i.e. $U \Delta_g U^* = \Delta_0 + A_0$, where $A \in \Psi^0(S^2)$. Here and henceforth, $\Psi^m(M)$ denotes the class of mth order pseudo-differential operators on a manifold M. Starting with any quantization one can improve it by an infinite sequence of pseudo-differential quantizations so that A_g commutes with Δ_g. The images $\{U\varphi_{k,q}^\gamma\}$ of the Gaussian beams for Δ_0 are then Gaussian beam eigenfunctions for $\mathcal{R}^2 = \Delta_g - A_0$.

The global quantum Birkhoff normal form is the statement that,

$$\sqrt{\Delta_g} = \mathcal{R} + A_{-1}, \text{ or equivalently } \Delta_g = \mathcal{R}^2 + A_0 \tag{2}$$

where $\mathcal{R}$ has the eigenvalues $k + \frac{1}{2}$ with multiplicity $2k+1$ (just as for the standard sphere), and where A_{-1} (resp. A_0) is a pseudo-differential operator of order -1 (resp. zero) commuting with $\mathcal{R}$ [**G**, **W**]. This commutation implies that the symbol $\sigma_{A_{-1}}$ of A_{-1} (resp. σ_{A_0} of A_0) is invariant under the geodesic flow. We may then interpret it as a function H on the space $G(S^2, g)$ of geodesics of the Zoll

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surface. The eigenvalues of A_{-1} in the kth cluster (where $\mathcal{R} = k+\frac{1}{2}$) have the form $\mu_k(q)$ where $q = -k, \dots, k$. Thus the spectrum of $\sqrt{\Delta_g}$ is a small perturbation $k + \frac{1}{2} + \mu_k(q)$ of that of the standard metric. The eigenvalue distribution of A_{-1} is determined by the function H. Explicit formulae are given in [**Z1**, **Z3**]. In effect we give yet another formula in this article.

1.1. Maximally degenerate Laplacians. A Laplacian of a surface is called *maximally degenerate* (in the sense of [**Z1**]) if the multiplicities of the distinct eigenvalues of the Laplacians are identical to the multiplicities $(1, 3, 5, \dots, 2k+1 \dots)$ of the eigenvalues $k(k+1)$ of the Laplacian for the standard metric on S^2. It is proved in [**Z1**] that in dimension 2, the metrices of MDL (maximally degenerate Laplacian) metrics must be Zoll metrics on S^2. Further it is proved that A_{-1} and A_0 in (2) are smoothing operators. The main question is whether any non-standard MDL Zoll Laplacians exist [**Y**]. It is known that the standard metric is the only MDL among surfaces of revolution [**E**, **Z1**]. But most Zoll metrics are not S^1 invariant. There exists an infinite dimensional moduli space of Zoll metrics, whose tangent space at the standard metric is isomoprhic to the space of odd functions on S^2.

The question whether there exist non-standard maximally degenerate Zoll Laplacians is of interest (to the author) because it is a very simple inverse spectral problem to state, yet defies most of the known techniques, and in some sense is a test for the strength of these techniques. The same question may be posed in higher dimensions, and then it is not even known if the standard metric on S^n is determined by its eigenvalues (with multiplicities) if $n \geq 7$. It has been proved that the standard metric on S^n is locally determined by its spectrum and therefore does not admit isospectral deformations. But it is not even known if the multiplicites of the eigenvalues of the standard S^2 are rigid, i.e. whether there exists a non-trivial Zoll deformation of the standard metric which preserves all of the eigenvalue multiplicities.

The relevance of Gaussian beams to this inverse problem is that, in the MDL case, Gaussian beams are eigenfunctions of the Laplacian. But the Gaussian beam construction involves an ansatz which leads to an eikonal equation and various transport equations. There exist obstructions to solving the transport equations, and they must vanish in the MDL case since Gaussian beams exist. The main purpose of this note is to explain how to write down such obstructions explicitly in terms of geometric invariants. The vanishing of the obstructions gives new conditions that an MDL must satisfy.

In fact, it was proved in [**Z1**] that the eigenvalues of an MDL Zoll surface agree with the standard eigenvalues $\ell(\ell+1)$ up to rapidly decaying errors. So the obstructions can be determined exactly. This idea is parallel to the strategy in [**Z2**], where the spectral projections $\Pi_\ell(x, y)$ kernels associated to the eigenspace were studied. If y is fixed, then $x \to \Pi_\ell(x, y)$ is the analogue of a zonal (rotationally invariant) eigenfunction on S^2 and may be viewed as a quasi-mode associated to the Lagrangian submanifold formed by meridian geodesics through the pole y. The obstructions to the Gaussian beam construction turn out to be quite different from the obstructions found in [**Z3**] to the construction of $\Pi_\ell(x, y)$.

Our main result, Theorem 1, states that if Δ_g is an MDL then the the integral over every closed geodesic γ of certain polynomials in the curvature and Jacobi fields must vanish. It turns out that the the polynomials are identical to the ones

that arise in the algorithm for constructing a quantum Birkhoff normal form for Δ around γ. In fact the normal forms algorithm and the algorithm for constructing Gaussian beams are equivalent and the obstructions are the same. They are simpler to compute in the normal forms algorithm and so after reviewing the Gaussian beam construction we mainly concentrate on normal forms.

1.2. Gaussian beams and Birkhoff normal form. To state the results, we first recall the construction of excited Gaussian beams along stable elliptic geodesics. We follow the exposition of [**BB**], which constructs Gaussian beams for every eigenvalue q of a transvese Harmonic oscillator. The qth excited Gaussian beam along an elliptic closed geodesic γ has the asymptotic form

$$\Phi_{kq}(s, \sqrt{r_{kq}}y) = e^{ir_{kq}s} \sum_{j=0}^{\infty} r_{kq}^{-\frac{j}{2}} U_q^{\frac{j}{2}}(s, \sqrt{r_{kq}}y, r_{kq}^{-1}). \tag{3}$$

In unscaled coordinates we denote them by φ_{kq}^{γ}. As recalled in §2, In the non-degenerate case, the semi-classical parameter r_{kq} has the form,

$$r_{kq} = k + \frac{1}{2} + \frac{1}{2\pi} \sum_{j=1}^{n} (q_j + \frac{1}{2})\alpha_j \tag{4}$$

where as above, $e^{i\alpha_j}$ are the eigenvalues of the Poincaré map P_γ. The coefficient functions $U^{\frac{j}{2}}$ are obtained by solving transport equations. The construction of $\Phi_{kq}(s, \sqrt{r_{kq}}y)$ produces a sequence of approximate eigenvalues associated to γ whose square roots have the semi-classical expansion

$$\lambda_{kq} \equiv r_{kq} + \frac{p_1(q)}{r_{kq}} + \frac{p_2(q)}{r_{kq}^2} + \dots \tag{5}$$

The numerators $p_n(q)$ are polynomials of specific degrees in q. We will express $p_n(q)$ as the eigenvalues of functions $p_n(I)$ where I are transvese Harmonic oscillators to γ, and will also consider the Weyl symbols $p_n(|z|^2)$ of $p_n(I)$. We will will show that $p_1(|z|^2)$ has the form $c_4|z|^4 + c_0$. It is not quite obvious that they are spectral invariants of Δ_g but in fact they are equivalent to the wave trace invariants along γ ([**G2**, **Z2**]).

Roughly speaking, one can write the transport equations in the form,

$$\frac{\partial}{\partial s}(\mu(a) U_q^{\frac{j}{2}}) = RHS, \tag{6}$$

where $\frac{\partial}{\partial s}$ is differentiation along γ and μ is a certain unitary transform. The obstruction to solving these equations is simply that $\int_\gamma (\text{RHS})\, ds = 0$. As we found in [**Z1**, **Z2**] (and will review below), the RHS is a complicated polynomial in the curvature τ, its normal derivatives τ_ν along γ and in the normal Jacobi fields $Y = y\nu$ along γ. Here ν is the unit normal frame along γ.

In the Zoll case, there exists a normal form for $\Delta_g - A_g$ and all of the subprincipal terms vanish. One has $\alpha_j = 0$ and so

$$r_{kq} = k + \frac{1}{2}$$

for all k, q. Similarly, one can construct Gaussian beams along any closed geodesic satisfying

$$(\Delta_g - A_0 + (k + \frac{1}{2})^2)\varphi_k^{\gamma} = O(k^{-\infty}),$$

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which implies that

$$(\Delta_g + (k+\frac{1}{2})^2)\varphi_k^\gamma = O(1), \ \ (k \to \infty).$$

There is already an obstruction to constructing such quasi-modes of order $O(1)$ of the form

$$\int_\gamma y^3 \tau_\nu dt \equiv 0, \ \ (\forall \gamma), \tag{7}$$

where $y\nu$ is a normal Jacobi field along γ. It is the simplest example of an obstruction (6). But the idenity holds for any geodesic of any Zoll surface as a result of Jacobi's equation (see (4.21) of [**Z1**]). This fact is an early indication of why the construction of Gaussian beams is possible on Zoll surfaces.

The principal symbol H of A_0 can be obtained as the limit,

$$H(\gamma) = \lim_{k\to\infty} \langle A_0 \varphi_k^\gamma, \varphi_k^\gamma \rangle.$$

The limit only involves the ground state $q = 0$ Gaussian beams. One may obtain 'higher symbols' by studying the limit along pairs (k, q) with $\frac{q}{k} \to \alpha$. We refer to [**UZ**] for some results in this direction. Viewed as a function on the space of geodesics $\simeq G(S^2, g)$, the eigenvalues $\mu_k(q)$ are roughly the values of H on the qth Bohr-Sommerfeld level with Planck constant $\frac{1}{k}$. The proof is based on putting H into Birkhoff normal form (i.e. express it in terms of local action variables) and is in some sense related to the quantum normal form of this article.

In the MDL case one may construct Gaussian beams which are exact eigenfunctions with eigenvalue $k(k+1) + S(k)$ where $S(k)$ is rapidly decaying. This leads to many further vanishing obstructions of the type (7). One must separate out integral formulae that hold universally on Zoll surfaces from ones which put extra conditions on g in the MDL case.

1.3. Constraints on maximally degenerate Zoll metrics. It is shown in [**Z1**, **Z3**] that, in the maximally degenerate Zoll case, all $p_j(q)$ in (5) are independent of q and depend only on k. In dimension 2, all of the terms below r_{kq} in the expansion (5) are zero. More precisely, we have

PROPOSITION 1. [**Z1**, **Z3**]

For a maximally degenerate Zoll surface, A_{-1} in (2) *is a smoothing operator, and there exists for each $q = 0, 1, 2 \cdots$ a sequence of Δ-eigenfunctions with the asymptotic form* (3). *The associated eigenvalues have the expansions* (5) *with $r_{kq} = (k+\frac{1}{2})$ and with all $p_n(q) = 0$. Thus, for every closed geodesic, $\lambda_{kq} = k(k+1)+S(k)$ where $S(k)$ is rapidly decaying.*

This puts an infinite number of additional constraints on a Zoll metric in the form of vanishing integrals over every closed geodesic of certain metric invariants. The simplest non-universal one is given in

THEOREM 1. *Let g be a Zoll metric on S^2. Then a necessary and sufficient condtion for existence of Gaussian beams* (3) *satisfying*

$$(\Delta_g - A_0 + (k+\frac{1}{2})^2)\Phi_{kq}^\gamma = O(k^{-2}), \ \ (k \to \infty)$$

along γ is that $p_1(q) = 0$ for all closed geodesics. At the closed geodsic $\gamma(t)$ with $t \in [0, \pi]$, the coefficients c_j $(j = 0, 2)$ of the Weyl symbol $p_1(|z|^2) = c_2|z|^4 + c_0$ of

$p_1(I)$ are given by the Weyl symbol σ_{A_0} plus

(8)

$$\tfrac{1}{2\pi}\int_0^{2\pi}[a_j|\dot{Y}|^4 + b_{1j}\tau|\dot{Y}Y|^2 + b_{2j}\tau\Re(\bar{Y}\dot{Y})^2 + c_j\tau^2|Y|^4 + d_j\tau_{\nu\nu}|Y|^4 + e_j\delta_{j0}\tau]ds$$

$$+\tfrac{1}{2\pi}\sum_{0\le m,n\le 3;m+n=3} C_{2;mnj}\Im\{\int_0^{2\pi}\tau_\nu(s)\bar{Y}^m Y^n(s)[\int_0^s \tau_\nu(t)\bar{Y}^n Y^m](t)dt]ds\}.$$

Here, Y is the complex periodic normal Jacobi field on γ with $Y(0) = 1, Y'(0) = i$, and $a_j, b_{1j}, b_{2j}, c_j, d_j, e_j, C_{2;mnj}$ are certain universal non-zero constants which depend on the index j. One has $e_j = 0$ if $j = 2$ and $d_j = 0$ if $j = 0$.

In the MDL case the integrals (8) *vanish for all γ.*

In fact, there are many further integrals of the same kind which must vanish in the MDL case.

We emphasize that the normal form exists for $\Delta_g - A_g = \mathcal{R}(\mathcal{R}+1)$. They can be used to determine the complete symbol of A_g. However, the emphasis of this note is on the MDL case and we do not consider general Zoll surfaces in detail.

Below we give a detailed algorithm for determining the terms and the universal coefficients. However it is rather technical and messy and it useful to have indirect checks on the calculations. In the case of the round metric, $\tau \equiv 1$ and the condition simplifies to

$$\tfrac{1}{2\pi}\int_0^{2\pi}[a|\dot{Y}|^4 + b_1|\dot{Y}Y|^2 + b_2 Re(\bar{Y}\dot{Y})^2 + c|Y|^4 + e\delta_{j0}]ds = 0.$$

Setting $y = e^{it}$ gives a universal linear relation among the universal constants in the formula for $j = 0, 2$.

For MDL's, $p_n(q) = 0$ for all n and all γ and that gives an infinite sequence of identities involving ever more derivatives which must vanish along every closed geodesic. Unfortunately the formulae for the higher polynomials $p_n(q)$ of (5) rapidly become extremely complicated. In the inverse spectral theory of bounded plane domains one can sift out spectral invariants by iterating, i.e. by replacing γ by its kth iterate γ^k. But in the Zoll case the integrand is periodic and iterating does not seem to produce new invariants.

As will be discussed in §7 (see §7.3), there are relations among the terms in the above integral due to integral geometric identities on Zoll surfaces. The result above should be compared with other formulae in [**Z1**, **Z3**]. In Theorem 3 of [**Z1**] the principal symbol $\sigma_{A_{-1}} = H$ is evaluated at γ to equal a universal multiple of

(9)

$$H(\gamma) = \int_\gamma \left(\tau + \left[\frac{1}{3}\tau_\nu(s)y^3(s)\int_0^s \tau_\nu(t)J^3(t)dt - \tau_\nu(s)u^2(s)J(s)\int_0^s \tau_\nu u J^2 dt\right]\right) ds,$$

which is similar to the expression of Theorem 1 but is simpler in having no fourth degree terms in the Jacobi fields. Here, u is the Jacobi fields with $u(0) = 1, \dot{u}(0) = 0$ and J is the area density in normal coordinates, which is essentially the Jacobi field with $J(0) = 0, \dot{J}(0) = 1$. The integral is obtained by regularizing $\int_\gamma J^{\frac{1}{2}}\Delta J^{-\frac{1}{2}}ds$.

In our view, the universal coefficients cannot be calculated reliably without a computer, and therefore we do not try to use the exact expression in Theorem 1 to draw conclusions in inverse spectral theory. Instead we rely on indirect arguments and on multiple calculations of the same quantity using different techniques. For instance the calculation of (9) in [**Z3**] is quite independent of Theorem 1 and suggests that there exist cancellations in the terms for $j = 0$. As reviewed in §7 the calculation in [**Z3**] is based on the construction of 'zonal quasi-modes' or spectral

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projections kernels in the MDL case. Unlike the Gaussian beam construction, where one constructs $\Phi_{k,q}^{\gamma}$ for all γ, q, we only considered the exact projection kernel and not a family of quasi-modes depending on the same Lagrangian submanifold, which might require a normal form along the Lagrangian.

1.4. Normal form invariants. The expression in Theorem 1 is the quantum Birkhoff normal form of degree 2 (i.e. $p_1(q)$ in (5)) and was calculated in [**Z2**] for a non-degenerate elliptic closed geodesic. In the non-degenerate case there are some additional terms which vanish in the Zoll case. In [**Z2**] we proved (in the non-degenerate case):

QBNF coefficients for k=0, dim =2 *$p_1(q)$ is given in complex Fermi normal coordinates $z = y + i\eta$ as $B_{0;4}|z|^4 + B_{0;0}$ where $B_{0;j}$ are given for both $j = 0, 4$ by polynomials in the normalized orthogonal Jacobi eigenvectors Y of P_γ by*

$$B_{0;j} = \frac{1}{L}\int_0^L [a|\dot{Y}|^4 + b_1\tau|\dot{Y}Y|^2 + b_2\tau Re(\bar{Y}\dot{Y})^2 + c\tau^2|Y|^4 + d\tau_{\nu\nu}|Y|^4 + e\delta_{j0}\tau]ds +$$

$$+\frac{1}{L}\sum_{0\leq m,n\leq 3; m+n=3} C_{1;mn}\frac{\sin((n-m)\alpha)}{|(1-e^{i(m-n)\alpha})|^2}|\int_0^L \tau_\nu(s)\bar{Y}^m Y^n](s)ds|^2$$

$$+\frac{1}{L}\sum_{0\leq m,n\leq 3; m+n=3} C_{2;mn} Im\{\int_0^L \tau_\nu(s)\bar{Y}^m Y^n(s)[\int_0^s \tau_\nu(t)\bar{Y}^n Y^m](t)dt]ds\}.$$

As mentioned above, the coefficients $C_{1;mn}$ and $C_{2;mn}$ are universal and come from commutator identities in the Weyl calculus (see §4.3). In dimension 2, and in the non-degenerate case, the space of complex normal Jacobi fields is spanned by the normalized eigenvectors $\{Y, \bar{Y}\}$.

The coefficient of the middle term of the normal form in the non-degenerate elliptic case would blow up in the Zoll case. Nevertheless the normal form exists in every Zoll case. The resolution is that the corresponding coefficient automatically vanishes for every closed geodesic. In the case of the second normal form invariant, the bad coefficient is (7) and vanishes for every Zoll surface.

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2. Jacobi fields and Poincaré map on a Zoll manifold

In this section we review the properties of Jacobi fields on Zoll manifolds. Let γ be a closed geodesic of length L_γ of a Riemannian manifold (M, g). We denote by $\mathcal{J}_\gamma^\perp \otimes \mathbb{C}$ the space of complex normal Jacobi fields along γ, a symplectic vector space of (complex) dimension 2n (n=dim M-1) with respect to the Wronskian

$$\omega(X, Y) = g(X, \frac{D}{ds}Y) - g(\frac{D}{ds}X, Y). \tag{10}$$

The linear Poincare map P_γ is the symplectic map on $\mathcal{J}_\gamma^\perp \otimes \mathbb{C}$ defined by

$$P_\gamma Y(t) = Y(t + L_\gamma).$$

The closed geodesic is *elliptic* if the eigenvalues of P_γ are of the form $\{e^{\pm i\alpha_j}, j = 1, \dots, n\}$. The associated normalized eigenvectors will be denoted $\{Y_j, \overline{Y_j}, j = 1, \dots, n\}$,

$$P\gamma Y_j = e^{i\alpha_j} Y_j \qquad P_\gamma \overline{Y}_j = e^{-i\alpha_j} \overline{Y}_j \quad \omega(Y_j, \overline{Y}_k) = \delta_{jk} \tag{11}$$

and relative to a fixed parallel normal frame $e(s) := (e_1(s), \dots, e_n(s))$ along γ they will be written in the form $Y_j(s) = \sum_{k=1}^n y_{jk}(s) e_k(s)$. As mentioned in the introduction, it is usually assumed in normal forms or Gaussian beams constructions that γ is non-degenerate elliptic, i.e. $\{\alpha_j, j = 1, \dots, n\}$ together with π, are independent over $\mathbf{Q}$.

In this article, we mainly consider surfaces, in which case $\mathcal{J}_\gamma^\perp \otimes \mathbb{C}$ has complex dimension two and as mentioned above is spanned by the eigenvectors $\{Y, \bar{Y}\}$. A normal Jacobi field along γ is simply of the form $Y(s) = y(s)\nu(s)$, where $\nu(s)$ is the parallel unit normal vector γ. Jacobi's equation is then a second order scalar equation,

$$y'' + \tau y = 0.$$

There is a two dimensional space of solutions: the vertical Jacobi field y_1 with initial conditions $y(0) = 0, y'(0) = 1$ and the horizontal Jacobi field y_2 with initial conditions $y(0) = 1, y'(0) = 0$ with respect to a fixed choice of origin $\gamma(0)$ of γ. We consider the pair (y, y') and form the symplectic Wronskian matrix:

$$a_s := \begin{pmatrix} y_2'(s) & y_1'(s) \\ y_2(s) & y_1(s) \end{pmatrix}. \tag{12}$$

We modify the Wronskian matrix so that its columns are given in terms of the normalized eigenvectors (11) of the Poincaré map:

$$\mathcal{A}(s) := \begin{pmatrix} \Im \dot{Y} & \Re \dot{Y} \\ \Im Y & \Re Y \end{pmatrix}. \tag{13}$$

The somewhat strange positioning of the elements is to maintain consistency with our reference [**Fo**] on the metaplectic representation.

In the Zoll case, $P_\gamma = Id$, i.e. the normal Jacobi fields are periodic (all $\alpha_j = 0$) and the Wronskian matrices a_s resp. $\mathcal{A}(s)$ are periodic. The a_s matrix is uniquely determined but $\mathcal{A}(s)$ is not since all normal Jacobi fields are eigenvectors of eigenvalue 1. We may thus assume

$$Y = y_1 + iy_2, \tag{14}$$

so that $a_s = \mathcal{A}(s)$.

Since we have a family of closed geodesics, we may differentiate with respect to the family. If we deform the geodesic in the direction of its unit normal, we obtain the variation y_ν, which satisfies (cf. [**Z1**], p. 573)

$$y_\nu'' + \tau_\nu y^2 + \tau y_\nu = 0. \tag{15}$$

To see this, we let $\gamma_r(t)$ be the variation of γ defined by $y\nu$ and then consider the family of Jacobi fields $Y_r = y_r \nu_r$ along γ_r with $Y_0 = y\nu$. Since $y_r'' + \tau(\gamma_r(t)) y_r = 0$ we obtain the formula by differentiating with respect to r at $r = 0$ using that $\frac{d}{dr}|_{r=0}\gamma_r(t) = y(t)$. The notation y_ν is short for $\frac{d}{dr} y_r|_{r=0}$.

The following Lemma illustrates universal integral formulae on Zoll surfaces.

LEMMA 2.1. *On a Zoll surface, for any normal Jacobi fields $y\nu, y_2\nu$ one has $\int_\gamma \tau_\nu y^2 y_2 ds = 0$ for all closed geodesics γ.*

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PROOF. If we multiply (15) by y_2, integrate over γ and transfer the $\frac{d}{ds}$ derivatives from y_ν'' to y_2, then by Jacobi's equation $\int_\gamma (y_2'' y_\nu + \tau y_2 y_\nu) ds = 0$ and therefore (7) is a universal identity for Jacobi fields along geodesics of Zoll surfaces. □

2.1. Fermi normal coordinates. Fermi normal coordinates are the normal coordinates defined by the exponential map $\exp : N_{\gamma,\epsilon} \to T_\epsilon(\gamma)$ from a ball in the normal bundle of γ to a tube of radius ϵ around γ. Thus we write $(s, y) = \exp_{\gamma(s)} y \cdot \nu_{\gamma(s)}$, where $\nu(s)$ is a choice of unit normal frame along γ. We write the associated metric coefficients as $g_{00} = g(\partial_s, \partial_s), g_{0j} = 0$ and $g_{jk} = g(\partial_{y_j}, \partial_{y_k}) = 1$.

In Fermi coordinates along a geodesic, the field $\frac{\partial}{\partial s}$ is a horizontal Jacobi field pointing between nearby normal geodesics to γ and tangent to the wave fronts. Each $\frac{\partial}{\partial y_j}$ is a geodesic vector field. The volume density is given by $j = \sqrt{\det g}$. In dimension two, $j = ||\frac{\partial}{\partial s}||$.

3. Gaussiam beam quasi-modes

The main result of [**BB**, **Ra2**, **Ra3**] is the construction of quasi-modes of the form (3) along a non-degenerate stable elliptic closed geodesic. We write

$$U_{kq}(s, \sqrt{r_{kq}} y, r_{kq}^{-1}) = \sum_{j=0}^{\infty} r_{kq}^{-\frac{j}{2}} U_q^{\frac{j}{2}}(s, \sqrt{r_{kq}} y, r_{kq}^{-1}), \tag{16}$$

and seek $U_q^{\frac{j}{2}}$ so that (3) approximately solves the eigenvalue problem.

$$\Delta_y e^{i r_{kq} s} U_{kq}(s, \sqrt{r_{kq}} y, r_{kq}^{-1}) \sim \lambda_{kq} e^{i r_{kq} s} U_{kq}(s, \sqrt{r_{kq}} y, r_{kq}^{-1}) \tag{17}$$

The eigenvalues associated to γ have the semi-classical expansion (5) where r_{kq} is given by (4). We now review the construction, following [**BB**].

It is sometimes convenient to express the various functions in terms of the scaled coordinates $\mu = \sqrt{r_{kq}} y$. The ground state Gaussian beam is a locally defined function in Fermi normal coordinates (s, μ) along γ of the form,

$$U_0 = \frac{1}{\sqrt{\det Y}} e^{\frac{i}{2}\left(\langle P Y^{-1} \mu, \mu \rangle\right)}.$$

Here, Y is the matrix of Jacobi eigen-fields and P is the matrix whose columns are $\frac{dY_j}{ds}$. Thus, $P = Y', PY^{-1} = Y'Y^{-1}$ and

$$Y^* P - P^* Y = iI \quad Y^T P - P^T Y = 0.$$

Using transverse creation and annihilation operators one can construct higher excited states as Gaussian beams U_q where the subscript $q = 0, 1, 2, \dots$ denotes the 'transverse energy level', i.e. the energy level of a Hermite operator in the normal directions to γ. When $q = 0$, the $j = 0$ term is defined by

$$U_q^0 = U_0(s, \mu) = (\det Y(s))^{-1/2} e^{i \frac{1}{2} \langle \Gamma(s) \mu, \mu \rangle} \tag{18}$$

where $\Gamma(s) := \frac{dY}{ds} Y^{-1}$ (see [**Ra**, **BB**]). For higher q, the initial term U_q^0 is like the qth excited state of the transverse harmonic oscillator and is defined by

$$U_q^0 = \Lambda^q U_0,$$

where

$$\Lambda = \textstyle\sum_{k=1}^2 (i y_k D_{y_k} - \frac{dy_k}{ds} y_k) \quad \Lambda^* = \sum_{k=1}^2 (-i \overline{y}_k D_{y_k} - \overline{\frac{dy_k}{ds}} y_k)$$

are the transverse creation/annihilation operators adapted to γ. Write

$$U_r = \Lambda_1^{*r_1} \cdots \Lambda_m^{*r_m} U_0 = Q_r(\mu, s) U_0.$$

Here, $r = (r_1, \dots, r_m)$. When M is a surface, there is just one k index.

As we now indicate, U_{kq} and $U_q^{\frac{j}{2}}$ are obtained by solving a sequence of transport equations.

3.1. Semi-classical scaling. To determine the coefficients $U_q^{\frac{j}{2}}$ in (3), one rescales the Laplacian to convert (17) into a semi-classical expansion. It is convenient to replace Δ by the unitarily equivalent 1/2-density Laplacian

$$\Delta_{1/2} := j^{1/2} \Delta j^{-1/2},$$

which can be written in the form:

$$\Delta_{1/2} = j^{-1/2} \partial_s g^{00} J \partial_s j^{-1/2} + \sum_{ij=1}^n j^{-1/2} \partial_{y_i} g^{ij} J \partial_{y_j} j^{-1/2}$$

$$\equiv g^{00} \partial_s^2 + \Gamma^0 \partial_s + \sum_{ij=1}^n g^{ij} \partial_{u_i} \partial_{y_j} + \sum_{i=1}^n \Gamma^i \partial_{y_i} + \sigma_0.$$

From now on, we denote $\Delta_{\frac{1}{2}}$ simply by Δ.

In dimension 2,

$$-\Delta = J^{-1/2} \partial_s g^{00} J \partial_s J^{-1/2} + J^{-1/2} \partial_y J \partial_y J^{-1/2}$$

$$\equiv g^{00} \partial_s^2 + (\partial_s g^{ss}) \partial_s + \partial_y^2 + \sigma_0 = g^{00} \partial_s^2 + (\Gamma^s_{ss}) \partial_s + \partial_y^2 + \sigma_0$$

For simplicity of notation, we put

$$h_{kq} := (2\pi k + \sum_{j=1}^n (q_j + \frac{1}{2} \alpha_j))^{-1}.$$

We observe that in (3) the Gaussian beams are in scaled coordinates $\mu = \sqrt{h_{kq}}^{-\frac{1}{2}} y$,

$$\Phi_{kq}(s, h_{kq}^{-\frac{1}{2}} y) = e^{i \frac{s}{h_{kq} L}} U_{kq}(s, \sqrt{h_{kq}}^{-\frac{1}{2}} y, h_{kq})$$

and the eigenvalue problem (17) becomes

$$\Delta_u e^{\frac{i}{h_{kq} L} s} U_{kq}(s, h_{kq}^{-\frac{1}{2}} y, h_{kq}) = \lambda(h_{kq}) e^{\frac{i}{h_{kq} L} s} U_{kq}(s, h_{kq}^{-\frac{1}{2}} y, h_{kq}).$$

When indices are not needed we simply write $h = h_{kq}$.

We transfer the scaling from the unknown function U to the Laplacian using the unitary operators T_h and M_h

$$T_h(f(s,y)|ds|^{1/2}|dy|^{1/2}) := h^{-n/2} f(s, h^{-\frac{1}{2}} y)|ds|^{1/2}|dy|^{1/2}$$

$$M_h(f(s,y)|ds|^{1/2}|dy|^{1/2}) := e^{\frac{i}{hL} s} f(s,y)|ds|^{1/2}|dy|^{1/2}.$$

We easily see that:

$$\text{(19)} \qquad \begin{cases} T_h^* D_{y_j} T_h = h^{-\frac{1}{2}} D_{y_j} \\ \\ T_h^* y_i T_h = h^{\frac{1}{2}} y_i, \\ \\ M_h^* D_s M_h = ((hL)^{-1} + D_s). \end{cases}$$

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We then rescale an operator A by

$$A_h := T_h^* M_h^* A T_h M_h. \tag{20}$$

The rescaled Laplacian then has the form,

$$\begin{aligned} -\Delta_h &= -(h)^{-2} g^{00}_{[h]} + 2i(h)^{-1} g^{00}_{[h]} \partial_s + i(h)^{-1} \Gamma^0_{[h]} \\ &\quad + h^{-1}(\textstyle\sum_{ij=1}^n g^{ij}_{[h]} \partial_{y_i} \partial_{y_j}) + h^{-\frac{1}{2}} (\sum_{i=1}^n \Gamma^i_{[h]} \partial_{y_i}) + (\sigma)_{[h]}, \end{aligned}$$

the subscript $[h]$ indicating to dilate the coefficients of the operator in the form, $f_h(s,y) := f(s, h^{\frac{1}{2}} y)$. Expanding the coefficients in Taylor series at $h = 0$, we obtain the asymptotic expansion

$$\Delta_h \sim \sum_{m=0}^{\infty} h^{(-2+m/2)} \mathcal{L}_{2-m/2} \tag{21}$$

where $\mathcal{L}_2 = 1$, $\mathcal{L}_{3/2} = 0$ and where

$$\mathcal{L}_1 =: \mathcal{L} = 2[i\frac{\partial}{\partial s} + \frac{1}{2}\{\sum_{j=1}^n \partial^2_{y_j} - \sum_{ij=1}^n K_{ij}(s) y_i y_j\}]. \tag{22}$$

Here, K_{ij} are the sectional curvatures. When the dimension is two,

$$\mathcal{L} = D_s - \frac{1}{2}(D_y^2 + \tau(s) y^2).$$

The semi-classical eigenvalue problem $\Delta_h U(s,y,h) = \lambda(h) U(s,y,h)$ then becomes,

$$\left(\textstyle\sum_{m=0}^{\infty} h^{(-2+m/2)} \mathcal{L}_{2-m/2}\right) U(s,y,h) = \lambda(h) U(s,y,h)) \tag{23}$$

with

$$U(s,y,h) = \sum_{j=0}^{\infty} h^{\frac{j}{2}} U_q^{\frac{j}{2}}(s,y,h). \tag{24}$$

By construction,

$$\mathcal{L} U_q^0 = (q + \frac{1}{2}) U_q^0.$$

The remaining terms are determined by 'transport equations' (26) of the form,

$$\mathcal{L} U_q^{\frac{j}{2}} = \text{RHS}, \tag{25}$$

for a known RHS.

The equation for $U_q^{h_0}$ is then shown to take the form of a sequence of transport equations with respect to the 'parabolic operator' $\mathcal{L}$,

$$\mathcal{L} U_q^{h_0} = -\mathcal{L}_1 U_q^{h_0 - 1} - \cdots - \mathcal{L}_{h_0} U_q^0 =: \Psi_q^{h_0} U_0, \tag{26}$$

where $\Psi_q^{h_0}$ is a polynomial in y with smooth coefficients in s. We next recall how this works.

3.2. Gaussian beam obstructions. In this section, we outline the algorithm in [**BB**] for determining the numerators $p_n(q)$ in (5). They are chosen to make transport equations solvable. We do not give the algorithm in detail because the equivalent Birkhoff normal forms algorithm is more efficient, in that it works simultaneously for all q.

We express the right side of (26) in the form

$$\Psi_q^{h_0}(y,s)U_0 = \sum_{(r)} A_{qr}^{h_0} U_r(y,s), \tag{27}$$

where (by orthogonality),

$$A_{qr}^{h_0} = \frac{1}{r!(2\pi)^{m/2}} \int_{\mathbb{R}^m} \Psi_q^{h_0} U_0 \overline{U}_r d\mu.$$

It follows that

$$A_{qr}^{h_0}(s+L) = e^{i(\kappa_q - \kappa_r)} A_{qr}^{h_0}(s),$$

with

$$\kappa_q = -\sum_{j=1}^m (\frac{1}{2} + q_j)\alpha_j, \quad \kappa_r = -\sum_{j=1}^m (\frac{1}{2} + r_j)\alpha_j.$$

In the Zoll case, $A_{qr}^{h_0}$ is periodic. If h_0 is odd, we find that $A_{qq}^{h_0}(s) = 0$.

Write

$$U_q^{h_0}(y,s) = \sum_{(r)} B_{qr}^{h_0}(s) U_r = \Phi_q^{h_0}(y,s)U_0. \tag{28}$$

In order that $U_q^{h_0} e^{i\kappa_q s}$ be periodic it is sufficient that

$$B_{qr}^{h_0}(s+L) = B_{qr}^{h_0}(s) e^{i(\kappa_q - \kappa_r)}.$$

One has $\mathcal{L}U_r = 0$ and the transport equations (26) simplify to

$$2i\frac{d}{ds} B_{qr}^{h_0}(s) = A_{qr}^{h_0}(s). \tag{29}$$

When $B_{qq}^{h_0}$ is periodic the necessary and sufficient condition for solvability is

$$\int_0^L A_{qq}^{h_0} ds = 0.$$

The numerators $p_n(q)$ of (5) are chosen to make this equation hold.

Thus, to determine the explicit geometric obstructions we would need to calculate $A_{qq}^{h_0}$ explicitly, and this is quite messy. We therefore turn to the normal forms construction, which calculates the same obstructions in a somewhat simpler way.

4. Quantum Birkhoff normal form construction

In this section we review the quantum normal form construction from [**Z2**]. As mentioned above, in the standard algorithm it is assumed there that the closed geodesic γ is non-degenerate elliptic. In this article, we want to understand why the algorithm still works in the Zoll case and how it must be modified. The modifications are emphasized in remarks.

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Let us summarize the key points of the normal form construction. The goal is to conjugate $\sqrt{\Delta}$ microlocally around γ to a function of the tangential operator $D_s := \frac{\partial}{i\partial s}$ along γ together with the transverse harmonic oscillators

$$I_j = I_j(y, D_y) := \frac{1}{2}(D_{y_j}^2 + y_j^2).$$

Here, (s, y) are Fermi normal coordinates along γ. We assume that the length L of γ equals 2π. Given the Floquet exponents, we form the operator

$$\mathcal{R} = D_s + H_\alpha$$

where

$$H_\alpha := \frac{1}{2}\sum_{k=1}^{n} \alpha_k I_k.$$

REMARK 4.1. *In the Zoll case, $H_\alpha = 0$ is zero and hence the Zoll Laplacian is conjugated to a function of D_s alone.*

In the non-degenerate case one has ([**Z2**]):

THEOREM 4.2. *There exists a microlocally elliptic Fourier Integral operator W from a conic neighborhood of $\mathbb{R}^+\gamma$ in $T^*N_\gamma - 0$ to a conic neighborhood of $T^*_+S^1$ in $T^*(S^1 \times R^n)$ such that:*

$$W\sqrt{\Delta_\psi}W^{-1} \equiv [\mathcal{R} + \frac{p_1(I_1, \dots, I_n)}{\mathcal{R}} + \frac{p_2(I_1, \dots, I_n)}{(\mathcal{R})^2} + \cdots + \frac{p_{k+1}(I_1, \dots, I_n)}{(\mathcal{R})^{k+1}} + \dots]$$

$$\equiv D_s + H_\alpha + \frac{\tilde{p}_1(I_1, \dots, I_n)}{D_s} + \frac{\tilde{p}_2(I_1, \dots, I_n)}{(D_s)^2} + \cdots + \frac{\tilde{p}_{k+1}(I_1, \dots, I_n)}{(D_s)^{k+1}} + \dots$$

where the numerators $p_j(I_1, \dots, I_n), \tilde{p}_j(I_1, \dots, I_n)$ are polynomials of degree j+1 in the variables $I_1, \dots, I_n$.

As explained in detail in [**Z2**], the $\equiv$ sign refers to a doubly-graded class $O_m\Psi^r$ of operators (or symbols). Here, Also, $O_m\Psi^r$ denotes the space of pseudodifferential operators of order r whose complete symbols vanish to order m at $(y, \eta) = (0, 0)$. The kth remainder term of the right sides of Theorem 4.2 lie in the space $\bigoplus_{j=0}^{k+2} O_{2(k+2-j)}\Psi^{1-j}$.

The polynomials are the same as the numerators of (5). We now go over the normal form algorithm in the non-degenerate case. We then consider how to modify it so that it produces a normal form for a Zoll Laplacian and in particular for am maximally degenerate one.

4.1. Metaplectic Jacobi conjugation. We work inductively on the semi-classical expansion (21). The first step is to put $\mathcal{L}$ (22) into normal form along γ. We do this by using a "moving metaplectic conjugation".

Let μ denote the metaplectic representation (see [**Fo**] for background). We apply μ to the matrix (13) of Jacobi fields to obtain,

$$\mu(\mathcal{A}) := \int_\gamma^\oplus \mu(\mathcal{A}(s))ds$$

on $\int_{S^1}^\oplus L^2(\mathbb{R}^n)ds = \int_\gamma^\oplus L^2(N_{\gamma(s)})ds$. In other words,

$$\mu(\mathcal{A})f(s, y) = \mu(\mathcal{A}(s))f(s, y)$$

where the operator on the right side acts in the y-variables. This conjugation simplifies the quadratic term (22) of the semi-classical expansion (21).

PROPOSITION 4.3. *The image $\mathcal{L}$ of D_s under μ is the operator* (22)*:*

$$\mathcal{L} := \mu(\mathcal{A})^* D_s \mu(\mathcal{A}) = D_s - \frac{1}{2}(\sum_{j=1}^n D_{y_j}^2 + \sum_{ij=1}^n K_{ij}(s) y_i y_j).$$

The relation of this conjugation to the Gaussian beam construction is as follows:
(i)

$$\mu(\mathcal{A}^{-1})\gamma_0(s,y) := U_0(s,y) = (\det Y(s))^{-1/2} e^{i\frac{1}{2}\langle \Gamma(s) y, y\rangle}$$

where $\Gamma(s) := \frac{dY}{ds} Y^{-1}$.
(ii) If γ_q denotes the q Hermite function, then

$$\mu(\mathcal{A}^{-1})\gamma_q := U_q = \Lambda_1^{q_1} \dots \Lambda_n^{q_n} U_0.$$

Lemma 4.3 shows that the first non-trivial term of (21) simplifies if we conjugate by $\mu(a)$. We therefore conjugate the entire expansion. We denote the new operators by

$$\begin{aligned} \mathcal{D}_h &= \mu(\mathcal{A})^{-1} \Delta_h \mu(\mathcal{A}) \\ &\sim \sum_{m=o}^\infty h^{(-2+\frac{m}{2})} \mathcal{D}_{2-\frac{m}{2}} \end{aligned} \tag{30}$$

with $\mathcal{D}_2 = I, \mathcal{D}_{\frac{3}{2}} = 0, \mathcal{D}_1 = D_s$.

This conjugation will make the transport equations take the form $D_s \mathcal{D}_p = \text{RHS}$ and thus easy to solve. On the other hand, for explicit calculations we need to use the $\mathcal{L}_q$'s.

4.2. Microlocal conjugation. We now microlocally conjugate (30) to the Birkhoff normal form of Theorem 4.2. The intertwining opertor in [**Z2**] has the form,

$$W_h := \mu(\mathcal{A})^* \prod_{k=1}^\infty W_{h\frac{k}{2}} \mu(a) \tag{31}$$

with

$$W_{h\frac{k}{2}} := \exp(ih^{\frac{k}{2}} Q_{\frac{k}{2}}).$$

Here, $Q_{\frac{k}{2}}$ is a polynomial differential operator which is constructed simultaneously with the normal form.

As discussed in [**Z2**], the $Q_{\frac{j}{2}}$ are constructed so that the conjugation removes all terms in the expansion (30) except for functions of the actions I_j. The procedure is algebraic, and is simplified by using the Weyl calculus because of its equivariance under metaplectic conjugation.

Each time we conjugate by one more factor of (31), we change the terms of the expansion (30), and we need to introduce some notation for the new expansions. We only carry out the algorithm to two orders. The first conjugation (by $\exp(ih^{\frac{1}{2}} Q_{\frac{1}{2}})$) produces

$$\begin{aligned} \mathcal{D}_h^{\frac{1}{2}} : &= \tilde{W}_{h\frac{1}{2}}^* \mathcal{D}_h \tilde{W}_{h\frac{1}{2}} \sim \sum_{n=0}^\infty h^{-2+\frac{n}{2}} \sum_{j+m=n} \frac{i^j}{j!} (ad\tilde{Q}_{\frac{1}{2}})^j \mathcal{D}_{2-\frac{m}{2}} \\ &= h^{-2} L^{-2} + h^{-1} L^{-1} D_s + \sum_{n=3}^\infty h^{-2+\frac{n}{2}} \mathcal{D}_{2-\frac{n}{2}}^{\frac{1}{2}}. \end{aligned}$$

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We then conjugate once more with $\tilde{W}_{h1} = e^{ih\tilde{Q}_1}$, to define

$$\mathcal{D}_h^1 := \tilde{W}_{h1}^* \mathcal{D}^{\frac{1}{2}} \tilde{W}_{h1} = h^{-2}L^{-2} + h^{-1}L^{-1}D_s + h^{-\frac{1}{2}}\mathcal{D}_{\frac{1}{2}}^{\frac{1}{2}} + \mathcal{D}_0^1(s, D_s, x, D_x) + \dots,$$

Thus, the superscript of $\mathcal{D}_b^a$ indexes the last factor of (31) used in the conjugation and the subscript is the opposite of the power of h, $h^{-2+\frac{n}{2}}$.

4.3. Commutators and Weyl symbols. In the Weyl calculus, commutators are given symbolically by the odd expansion

$$a\#b - b\#a \sim \frac{1}{i}P_1(a,b) + \frac{1}{i^3 3!}P_3(a,b) + \dots$$

while anticommutators involve only the even transvectants. One easily computes that

$$P_1(z^m\bar{z}^n, z^\mu\bar{z}^\nu) = C_{1;mn\mu\nu} z^{m+\mu-1}\bar{z}^{n+\nu-1}$$

where $C_{1;mn\mu\nu} = \frac{1}{2}\sigma((m,n),(\mu,\nu))$ with σ the standard symplectic inner product, and that

$$P_3(z^m\bar{z}^n, z^\mu\bar{z}^\nu) = C_{(m,n),(\mu,\nu)} z^{m+\mu-3}\bar{z}^{n+\nu-3}$$

for certain other coefficients $C_{(m,n),(\mu,\nu)}$. These are the C-coefficients in Theorem 1.

4.4. First odd term. To begin with, we construct $Q_{\frac{1}{2}}$ so that conjugation by $\exp(ih^{\frac{1}{2}}Q_{\frac{1}{2}})$ removes $\mathcal{D}_{\frac{1}{2}}$ in (30), i.e. so that $\mathcal{D}_{\frac{1}{2}}^{\frac{1}{2}} = 0$. This happens if $Q_{\frac{1}{2}}$ solves the *homological equation*

$$\{i[D_s, \mu(r_\alpha)^* Q_{\frac{1}{2}}\mu(r_\alpha)] + \mathcal{D}_{\frac{1}{2}}\}|_0 = 0,$$

or equivalently,

$$\partial_s\{\mu(r_\alpha)^* Q_{\frac{1}{2}}\mu(r_\alpha)\}|_0 = -i\{\mathcal{D}_{\frac{1}{2}}\}|_0. \tag{32}$$

Here,

$$r_{\alpha_j}(s) := \begin{pmatrix} \cos\alpha_j\frac{s}{L} & \sin\alpha_j\frac{s}{L} \\ -\sin\alpha_j\frac{s}{L} & \cos\alpha_j\frac{s}{L} \end{pmatrix}. \tag{33}$$

where L is the length of γ. Since our main application is to Zoll surfaces, where the closed geodesics all have the same primitive period [**GrGr**], we usually set $L = 2\pi$ or 1 to simplify notation. In the Zoll case they are the same. Also, "$A|_0$" denotes restriction of a pseudo-differential operator A on $S^1 \times \mathbb{R}^n$ to elements in the kernel of $\mathcal{R}$. Equivalently, after conjugation by $\mu(r_\alpha)$, to elements in the kernel of D_s, that is, to functions independent of s. Thus, if $A = A_2D_s^2 + A_1D_s + A_0$, then $A|_0 = A_0|_0$.

To solve (32), we rewrite it in terms of complete Weyl symbols. We denote by $A(s,x,\xi)$ the complete Weyl symbol of the operator $A(s,x,D_x)$. Then (32) becomes

$$\partial_s\tilde{Q}_{\frac{1}{2}}(s,x,\xi) = -i\mathcal{D}_{\frac{1}{2}}|_0(s,x,\xi) \tag{34}$$

with

$$\tilde{Q}_{\frac{1}{2}}(s+L,x,\xi) = \tilde{Q}_{\frac{1}{2}}(s, r_\alpha(L)(x,\xi)).$$

Here L is the length of γ (which we usually take to be 2π). We rewrite (34) in the integral form

$$\tilde{Q}_{\frac{1}{2}}(s,x,\xi) = \tilde{Q}_{\frac{1}{2}}(0,x,\xi) + L\int_0^s -i\mathcal{D}_{\frac{1}{2}}|_0(u,x,\xi)du \tag{35}$$

and then $\tilde{Q}_{\frac{1}{2}}(0,x,\xi)$ is determined by the consistency condition

$$\tilde{Q}_{\frac{1}{2}}(L,x,\xi) - \tilde{Q}_{\frac{1}{2}}(0,x,\xi) = L\int_0^L -i\mathcal{D}_{\frac{1}{2}}|_0(u,x,\xi)du.$$

or in view of the periodicity properties of Q, by

$$\tilde{Q}_{\frac{1}{2}}(0,r_\alpha(x,\xi)) - \tilde{Q}_{\frac{1}{2}}(0,x,\xi) = L\int_0^L -i\mathcal{D}_{\frac{1}{2}}|_0(u,x,\xi)du. \tag{36}$$

REMARK 4.4. *In the Zoll case, both sides of this equation must be zero and thus a solution of* (35) *is given by*

$$\tilde{Q}_{\frac{1}{2}}(s,x,\xi) = L\int_0^s -i\mathcal{D}_{\frac{1}{2}}|_0(u,x,\xi)du.$$

To solve (36), we change to complex coordinates $z_j = x_j + i\xi_j$ and $\bar{z}_j = x_j - i\xi_j$ in which the action of $a(s)$ or $r_\alpha(L)$ is diagonal. Then (34) becomes,

$$\tilde{Q}_{\frac{1}{2}}(0,e^{i\alpha}z,e^{-i\alpha}\bar{z}) - \tilde{Q}_{\frac{1}{2}}(0,z,\bar{z}) = \int_0^L -i\mathcal{D}_{\frac{1}{2}}|_o(u,z,\bar{z})du$$

We now use that $\mathcal{D}_{\frac{1}{2}}(u,z,\bar{z})$ is a polynomial of degree 3, and put

$$\tilde{Q}_{\frac{1}{2}}(s,z,\bar{z}) = \sum_{|m|+|n|\leq 3} q_{\frac{1}{2};mn}(s)z^m\bar{z}^n,\quad \mathcal{D}_{\frac{1}{2}}|_0(s,z,\bar{z})du = \sum_{|m|+|n|\leq 3} d_{\frac{1}{2};mn}(s)z^m\bar{z}^n \tag{37}$$

then (34) or (36) becomes

$$\sum_{|m|+|n|\leq 3}(1-e^{(m-n)\alpha})q_{\frac{1}{2};mn}(0)z^m\bar{z}^n = -i\sum_{|m|+|n|\leq 3}\bar{d}_{\frac{1}{2};mn}z^m\bar{z}^n. \tag{38}$$

Here, the bar in $\bar{d}_{\frac{1}{2};mn}$ denotes the time average over one period. The obstruction to solving this equation if the right side is non-zero is invertibility of the coefficients $(1-e^{(m-n)\alpha})$. Since there are no terms with $m=n$ in this (odd-index) equation, there is no obstruction to the solution of (38) if the α_j's are independent of π over $\mathbb{Z}$.

REMARK 4.5. *In the Zoll case, both sides of* (38) *equal zero by Lemma* 2.1 *(as mentioned above). We solve with* $q_{\frac{1}{2};mn}(s) = L\int_0^s d_{\frac{1}{2};mn}(s)ds$. *It follows that* $q_{\frac{1}{2};m,n}(0) = 0$.

4.5. First even term. Next we seek $\tilde{Q}_1$ so that conjugation by $\tilde{W}_{h1} = e^{ih\tilde{Q}_1}$ removes as much as possible of the first even term of the conjugate $\mathcal{D}_h^{\frac{1}{2}}$ of (30) by $\exp(ih^{\frac{1}{2}}Q_{\frac{1}{2}})$ in the previous step. This step becomes computationally involved since we need to conjugate (30) by $\exp(ih^{\frac{1}{2}}Q_{\frac{1}{2}})$ and introduce notation for the new terms. For simplicity of exposition we refer to [**Z2**] for the details of all the steps and just explain the notation for the first two conjugations.

In the second conjugation, we seek an element $\tilde{Q}_1(s,x,D_x)\in\Psi^*(S^1\times\mathbb{R}^n)$ and a function $f_0(I_1,\dots,I_n)$ of the Harmonic Oscillators so that

$$\mathcal{D}_h^1 := \tilde{W}_{h1}^*\mathcal{D}^{\frac{1}{2}}\tilde{W}_{h1} = h^{-2}L^{-2} + h^{-1}L^{-1}D_s + h^{-\frac{1}{2}}\mathcal{D}_{\frac{1}{2}}^{\frac{1}{2}} + \mathcal{D}_0^1(s,D_s,x,D_x) + \dots$$

with

$$\mathcal{D}_0^1(s,D_s,x,D_x)|_0 = f_0(I_1,\dots,I_n), \tag{39}$$

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Note that due to the choice of the first conjugation, $\mathcal{D}^1_{\frac12} = \mathcal{D}^{\frac12}_{\frac12} = 0$. We now choose the second $\tilde{Q}_1$ to remove as much as possible of the h^0 term, i.e. all of the "off-diagional" terms of the Weyl symbol of $\mathcal{D}^1_0$. First, we observe that

$$\mathcal{D}^1_0 = \mathcal{D}^{\frac12}_0 + i[D_s, \tilde{Q}_1].$$

Thus, we seek $\tilde{Q}_1$ so that

$$\{i[D_s, \tilde{Q}_1] + \mathcal{D}^{\frac12}_0\}|_0 = f_0(I_1, \dots, I_n).$$

or equivalently

$$\partial_s \tilde{Q}_1|_0 = \{-\mathcal{D}^{\frac12}_0 + f_0(I_1, \dots, I_n)\}|_0. \tag{40}$$

We further note that

$$\mathcal{D}^{\frac12}_0 = \mathcal{D}_0 + \frac{i}{2}[\mathcal{D}_{\frac12}, \tilde{Q}_{\frac12}]. \tag{41}$$

Recall here that $\mathcal{D}_{\frac12}$ is the term of order $h^{-\frac12}$ in (30) and that $\tilde{Q}_{\frac12}$ is accompanied by $h^{\frac12}$. There is an additional double commuator $[[D_s, \tilde{Q}_{\frac12}], \tilde{Q}_{\frac12}]$ term, but since $[D_s, \tilde{Q}_{\frac12}] = i\mathcal{D}_{\frac12}$ by the first step, we get

$$\frac{i}{2}[\mathcal{D}_{\frac12}, \tilde{Q}_{\frac12}] = i[\mathcal{D}_{\frac12}, \tilde{Q}_{\frac12}] - \frac{1}{2}[[D_s, \tilde{Q}_{\frac12}], \tilde{Q}_{\frac12}].$$

4.6. Solution of the second homological equation. We rewrite (40) in terms of complete Weyl symbols and obtain the second homological equation,

$$\partial_s \tilde{Q}_1(s, z, \bar{z}) = -i\{\mathcal{D}^{\frac12}_0|_0(s, z, \bar{z}) - f_0(|z_1|^2, \dots, |z_n|^2)\}$$

or equivalently

$$\tilde{Q}_1(s, z, \bar{z}) = \tilde{Q}_1(0, z, \bar{z}) - i\int_0^s [\mathcal{D}^{\frac12}_0|_0(u, z, \bar{z}) - f_0(|z_1|^2, \dots, |z_n|^2)]du$$

and solve simultaneously for $\tilde{Q}_1$ and f_0. The consistency condition determining a unique solution is that

$$\tilde{Q}_1(L, z, \bar{z}) = \tilde{Q}_1(0, z, \bar{z}) - i\int_0^L [\mathcal{D}^{\frac12}_0|_0(u, z, \bar{z}) - f_0(|z_1|^2, \dots, |z_n|^2)]du.$$

or

$$\tilde{Q}_1(0, e^{i\alpha}z, e^{-i\alpha}\bar{z}) - \tilde{Q}_1(0, z, \bar{z}) = -i\{\int_0^L \mathcal{D}^{\frac12}_0|_0(u, z, \bar{z})du - f_0(|z_1|^2, \dots, |z_n|^2)\}.$$

Now, $\mathcal{D}^{\frac12}_0|_0(u, z, \bar{z})$ is a polynomial of degree 4. Indeed, $\mathcal{D}_0(u, z, \bar{z})$ is a polynomial of degree 4, and the Weyl symbol of $[\mathcal{D}_{\frac12}, \tilde{Q}_{\frac12}]$ is also of degree since it is the Poisson bracket of polynomials of degree 3 (see §4.3). We assume that the Weyl symbol $\tilde{Q}_1(s, z, \bar{z})$ is a polynomial of degree 4. We put

$$\tilde{Q}_1(s, z, \bar{z}) = \sum_{|m|+|n|\le 4} q_{1;mn}(s) z^m \bar{z}^n, \qquad f_0(|z_1|^2, \dots, |z_n|^2) = \sum_{|k|\le 2} c_{0k}|z|^{2k}$$

and

$$\mathcal{D}^{\frac12}_0|_0(s, z, \bar{z})du := \sum_{|m|+|n|\le 4} d^{\frac12}_{0;mn}(s) z^m \bar{z}^n, \qquad \bar{d^{\frac12}_{0;mn}} := \frac{1}{L}\int_0^L d^{\frac12}_{0;mn}(s)ds.$$

The second homological equation thus becomes,

$$\begin{cases} \sum_{|m|+|n|\leq 4, m\neq n}(1-e^{i(m-n)\alpha})q_{1;mn}(0)z^m\bar{z}^n = \sum_{|m|+|n|\leq 4, m\neq n}\overline{d^{\frac{1}{2}}_{0;mn}}z^m\bar{z}^n, \\ \overline{d^{\frac{1}{2}}_{0;mm}} =: f_0(I). \end{cases} \tag{42}$$

In the non-degenerate case, we can solve for the off-diagonal coefficients,

$$q_{1;mn}(0) = -i(1-e^{i(m-n)\alpha})^{-1}\bar{d}^{\frac{1}{2}}_{0;mn}.$$

We cannot divide when $m = n$, and must set the diagonal coefficients equal to zero. The coefficients c_{0k} of f_0 (the normal form) are then determined by

$$c_{0k} = \bar{d}^{\frac{1}{2}}_{0;kk}.$$

It is evident that $\tilde{Q}_1$ and $f_0(I_1,\dots,I_n)$ are even polynomial pseudodifferential operators of degree 4 in the variables (x, D_x). The coefficients c_{0k} are essentially the QBNF invariants.

REMARK 4.6. *In the MDL Zoll case, the left side of the off-diagonal sum $m \neq n$ is zero, and therefore a necessary condition for solvability is that $\overline{d^{\frac{1}{2}}_{0;mn}} = 0$ for all $m \neq n$ with $m + n \leq 4$. In the maximally degenerate case, the normal form term f_0 is also zero and therefore we also have $\bar{d}^{\frac{1}{2}}_{0;kk} = 0$ for $k = 0, 1, 2$.*

Again we solve for $\tilde{Q}_1$ by direct integration,

$$q_{1;m,n}(s) = \int_0^s (d^{\frac{1}{2}}_{0;m,n}(s) - \delta_{mk}\delta_{nk}c_{0k}|z|^{2k})ds.$$

.

5. Maximally degenerate Zoll case

As we have remarked in the summary above, and the solvability of the homological equations is possible in the Zoll case where $(1-e^{i(m-n)\alpha}) = 0$ only when the right side of the homological equations vanish. In this section we review the results that prove that the normal form does exist and hence the homological equations are solvable when Δ_g is maximally degenerate. In the general Zoll case, one needs to subtract the operator A_0 to solve the equations and A_0 is determined by the solvability of the equations.

As mentioned in the introduction, it is proved in [**W**, **G**] that on any Zoll surface there exists a global unitary Fourier integral operator U intertwining Δ_g with the standard Laplacian modulo a remainder of order zero, i.e.

$$U\Delta U^* = \Delta_0 + A_0, \quad U\sqrt{\Delta}U^* = \sqrt{\Delta_0} + A_{-1}. \tag{43}$$

Thus, $\Delta_g - A_0$ has a complete degenerate global quantum Birkhoff normal form. It restricts around each closed geodesic to a microlocal one. Hence the homological equations must be solvable.

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5.1. Spectral projections and unitary intertwining operators in the MDL case. The unitary intertwining can be constructed directly in terms of Gaussian beams. First in the standard S^2, the spectral projection to the kth eigenspace $\mathcal{H}_k$ of spherical harmonics on S^2 of degree k satisfies the following identity,

$$\Pi_k(x,y) = \int_{G(S^2,g_0)} \varphi_k^\gamma \otimes \varphi_k^\gamma d\mu(\gamma).$$

Here, $G(S^2, g_0)$ is the symplectic space of geodesics and $d\mu(\gamma)$ is the symplectic area form. Also, φ_k^γ is the Gaussian beam (highest weight spherical harmonic) of degree k.

One then constructs Gaussian beams on any Zoll surface by $U^*\varphi_k^\gamma$, since

$$\Delta U^*\varphi_k^\gamma = U(\Delta_0 + Q_0)\varphi_k^\gamma = \lambda_0(q,h)U\varphi_k^\gamma + UQ_0\varphi_k^\gamma.$$

The second term is $\mathcal{O}(1)$. In general, $U^*\varphi_k^\gamma$ is only a quasi-mode of order zero.

The unitary intertwining operator U thus takes φ_k^γ to the ground state Gaussian beam $\psi_k^{\chi(\gamma)}$ for g along $\chi(\gamma)$ where $\chi : G(S^2, g_0) \to G(S^2, g)$ is a symplectic diffeomorphism. We therefore have,

PROPOSITION 5.1. *Let $\chi : G(S^2, g) \to G(S^2, g_0)$ be a symplectic diffeomorphism (1). Let (S^2, g) be MDL. Then, a unitary intertwining operator for the kth cluster is defined by*

$$U_k(x,y) = \int_{G(S^2,g_0)} \psi_k^{\chi(\gamma)} \otimes \varphi_k^\gamma d\mu(\gamma).$$

In the maximally degenerate case, this formula constructs U so that $U\varphi_k^\gamma$ is an eigenfunction of the Zoll surface.

5.2. Maximally degenerate Zoll Laplacians. We now specialize to the maximally degenerate case. It follows from Proposition 1 and Remark 4.6 that:

THEOREM 5.2. [**Z1**, **Z2**] *If (S^2, g) is a Zoll surface with a maximally degenerate Laplacian, then for every closed geodesic, all of the coefficents $p_j(I_1, I_2)$ and $\tilde{p}_j(I_1, I_2)$ equal zero. In particular, $A_{-1} = 0$ and $\overline{d^{\frac{1}{2}}_{k;mn}} = 0$ for all m, n with $m + n \leq 4$. Moreover, $\bar{d}^q_{m,n} = 0$ for all q and m, n.*

We now derive some explicit geometric consequences from Theorem 5.2, in particular Theorem 1, by calculating $d^{\frac{1}{2}}_{m,n}$. The diagonal calculations are essentially in [**Z2**] except that we need to clarify their solvability in the case of MDL Zoll surfaces. It appears that the vanishing of the off-diagonal coefficients gives yet futher constraints on g of the same form as in Theorem 1 but with different coefficients. This will become visible in the proof.

6. Explicit formulae on Zoll surfaces

We wish to evalute the coefficients $\overline{d^{\frac{1}{2}}_{m,m}}$ or equivalently the complete symbol of f_0 in terms of integrals over γ of Fermi-Jacobi data. At first, we will allow the dimension to be arbitrary; when it is time to substitute in metric expressions we will restrict to dimension 2.

6.1. Abstract calculation. To calculate $f_0(|z|^2)$, we need to unravel the diagonal part of the equation

$$\int_0^L \mathcal{D}_0^{\frac{1}{2}}|_0(u,z,\bar{z})du. \tag{44}$$

The integrand is given in (41) and consists of two terms $\mathcal{D}_0 + \frac{i}{2}[\mathcal{D}_{\frac{1}{2}}, \tilde{Q}_{\frac{1}{2}}]$. We first consider the commutator term. We note that $\mathcal{D}_{\frac{1}{2}}$ is independent of D_s so that $\mathcal{D}_{\frac{1}{2}}|_0 = \mathcal{D}_{\frac{1}{2}}$. It follows that

$$[\mathcal{D}_{\frac{1}{2}}(s), \tilde{Q}_{\frac{1}{2}}(s)] = [\mathcal{D}_{\frac{1}{2}}(s), \tilde{Q}_{\frac{1}{2}}(0)] + [\mathcal{D}_{\frac{1}{2}}(s), \int_0^s \mathcal{D}_{\frac{1}{2}}(t)dt]$$

so that the second term of (41) contributes to $f_0(I_1,\dots,I_n)$ the *diagonal part* of

$$\frac{i}{2}\{[\tilde{Q}_{\frac{1}{2}}(0, e^{i\alpha}z, e^{-i\alpha}\bar{z}), \tilde{Q}_{\frac{1}{2}}(0,z,\bar{z})] + \frac{1}{2}\{[\int_0^L \mathcal{D}_{\frac{1}{2}}(s)ds, \int_0^s \mathcal{D}_{\frac{1}{2}}(t)dt]. \tag{45}$$

Here, the bracket $[,]$ denotes the commutator of complete symbols in the sense of operator (or complete symbol) composition. In the Zoll case, $\tilde{Q}_{\frac{1}{2}}(0,\cdot,\cdot) = 0$ by Remark 4.5 and Remark 4.6. For emphasis:

REMARK 6.1. *In the Zoll case, $q_{\frac{1}{2};m,n}(0) = 0$ and therefore this commutator term is zero.*

6.2. Explicit calculations of obstruction integrals. To evaluate the expressions $\mathcal{D}_{\frac{1}{2}}$ and $\mathcal{D}_0$. we conjugate back to the $\mathcal{L}$'s:

$$\mathcal{D}_0 = \mu(\mathcal{A}^*)\mathcal{L}_0\mu(\mathcal{A}^*)^{-1}, \qquad \mathcal{D}_{\frac{1}{2}} = \mu(\mathcal{A}^*)\mathcal{L}_{\frac{1}{2}}\mu(\mathcal{A}^*)^{-1} \tag{46}$$

where as in (13),

$$\mathcal{A}(s) := \begin{pmatrix} \Im\dot{Y} & \Re\dot{Y} \\ \Im Y & \Re Y \end{pmatrix}. \tag{47}$$

REMARK 6.2. *As noted above, Y is uniquely defined in the non-degenerate case but not in the Zoll case. We return to this point in the next section.*

We then conjugate the symbols. By metaplectic covariance of the Weyl calculus, the conjugations change the complete Weyl symbols of the $\mathcal{L}$'s (in the x variables) by the linear symplectic transformation $\mathcal{A}$, i.e by the substitutions

$$\begin{array}{l} x \to [(\Re Y)x + (\Im Y)\xi] = \frac{1}{2}[\bar{Y}\cdot z + Y\cdot\bar{z}] \\ \xi \to [\Re\dot{Y}x + (\Im\dot{Y})\xi] = \frac{1}{2}[\dot{Y}\cdot z + \dot{Y}\bar{z}] \end{array}. \tag{7.8}$$

6.3. Dimension 2. In dimension 2 we have (in scaled Fermi coordinates)

$$\begin{aligned} g^{oo}(s,y) &= 1 + C_1\tau(s)y^2 + C_2\tau_\nu(s)y^3 + \dots \\ g^{11} &= 1 \\ J(s,u) &= \sqrt{g_{oo}} = 1 + C_1'\tau(s)y^2 + \dots \end{aligned}$$

for some universal (metric independent) constants C_j, C_j' which will change from line to line. They will end up in the the coefficients of the normal form.

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Using the Taylor expansion of the metric coefficients one finds that

LEMMA 6.3. *We have,*

$$\begin{cases} \mathcal{L}_{\frac{1}{2}} = CL^{-2}\tau_\nu(s)y^3, \\ \\ \mathcal{L}_0 = C_1L^{-2}y^4\tau_{\nu\nu} + C_2L^{-1}y^2\tau\partial_s + C_3L^{-1}\tau_s y^2 - \partial_s^2 + C_4\tau y\partial_y + C_5\tau. \end{cases}$$

All terms have weight -2.

We now complete the calculation of the diagonal terms in (44). We rewrite the commutators in terms of the coefficients (37) at $s = 0$ and the Poisson bracket constants in §4.3.

As noted in Remark 4.5,Remark 4.6 and Remark 6.1, $\tilde{Q}_{\frac{1}{2}}(0) = 0$ and therefore its commutators make no contribution in the Zoll case. Thus we only need to calculate the diagonal part of

$$\frac{1}{2}\{[\int_0^L \mathcal{D}_{\frac{1}{2}}(s)ds, \int_0^s \mathcal{D}_{\frac{1}{2}}(t)dt] + \mathcal{D}_0. \tag{48}$$

The diagonal part is the part which is a function only of $|z|^2$. The off-diagonal terms have not previously been studied because they can be eliminated from the normal form in the non-degenerate case. Their vanishing in the MDL Zoll case is additional information on the metric.

We now prove the following Lemma and also evaluate the coefficients:

LEMMA 6.4. *The diagonal part of* (48) *term has the form*

$$\textit{Diagonal Part}\left(\tfrac{1}{2}\int_0^L \int_0^s [\tilde{D}_{\frac{1}{2}}(s,z,\bar{z}), \tilde{D}_{\frac{1}{2}}(t,z,\bar{z}]dsdt\right) = A_4|z|^4 + A_0,$$

with

$$A_4 = [\int_0^L \int_0^s C_{1;3030}d_{\frac{1}{2};30}(s)d_{\frac{1}{2};03}(t) + C_{1;2112}d_{\frac{1}{2};21}(s)d_{\frac{1}{2};12}(t)$$

$$+C_{1;1221}d_{\frac{1}{2};12}(s)d_{\frac{1}{2};21}(t) + C_{1;0330}d_{\frac{1}{2};30}(s)d_{\frac{1}{2};03}(t)dsdt]$$

and with

$$A_0 = [\int_0^L \int_0^s [C_{3;3030}d_{\frac{1}{2};30}(s)d_{\frac{1}{2};03}(t)$$

$$+C_{3;2112}d_{\frac{1}{2};21}(s)d_{\frac{1}{2};12}(t) + C_{3;1221}d_{\frac{1}{2};12}(s)d_{\frac{1}{2};21}(t) + C_{3;0330}d_{03}(s)d_{\frac{1}{2};30}(t)]dsdt].$$

The coefficients are universal.

Making the linear symplectic substitutions above we first get

$$\mathcal{D}_{\frac{1}{2}}(s,z,\bar{z}) = C\tau_\nu(s)([\bar{Y}\cdot z + Y\cdot\bar{z}])^3. \tag{49}$$

We note that $\mathcal{D}_{\frac{1}{2}}(s)$ is a homogeneous polynomial of degree 3. Obviously,

LEMMA 6.5. *For $m+n=3$, the coefficient of $z^m\bar{z}^n$ in $\mathcal{D}_{\frac{1}{2}}(s)$ is*

$$d_{\frac{1}{2};mn}(s) = C_{mn;3}\tau_\nu[\bar{Y}^m\cdot Y^n](s).$$

Let $[F,G] = F\#G - G\#F$. Then the commutator in (48) equals

$$\sum_{m+n=3,p+q=3} C_{m,n,p,q} \left(\int_0^L \int_0^s d_{\frac{1}{2};mn}(s) d_{\frac{1}{2};pq}(t) ds dt \right) [z^m \bar{z}^n, z^p \bar{z}^q]$$

$$= \sum_{m+n=3,p+q=3} C'_{m,n,p,q} \{ [\int_0^L \tau_\nu(s) [\bar{Y}^m \cdot Y^n](s) \int_0^s \tau_\nu(t) [\bar{Y}^p \cdot Y^q](t) dt \} \tag{50}$$

$$\times [z^m \bar{z}^n, z^p \bar{z}^q].$$

The commutator $[z^m \bar{z}^n, z^p \bar{z}^q]$ is described in §4.3 and is a sum of a Poisson bracket and a third transvectant.

6.3.1. *Diagonal terms of the commutator.* We note that

$$\{z^m \bar{z}^n, z^p \bar{z}^q\} = C z^{m+p-1} \bar{z}^{n+q-1}$$

and since $\mathcal{D}_{\frac{1}{2}}$ is homogeneous of degree 3, to obtain a term of type $|z|^{2k}$ $(k = 0, 1, 2)$ we need $m + p = k + 1 = n + q, m + n = 3 = p + q$. The only non-zero Poisson bracket occurs when $k = 2$ and then $m + p = 3 = n + q$, so $p = n, q = m$. This produces terms of the form $[z^m \bar{z}^n, z^n \bar{z}^m]$ times

$$\{ [\int_0^L \tau_\nu(s) [\bar{Y}^m \cdot Y^n](s) \int_0^s \tau_\nu(t) [\bar{Y}^n \cdot Y^m](t) dt \}.$$

If we interchange $m \to n, n \to m$, the diagonal terms of the commutator $[z^m \bar{z}^n, z^n \bar{z}^m]$ changes sign and the above integral changes to its complex conjugate. Hence, the diagonal part of the commutator produces a sum of terms,

$$\sum_{m+n=3} C_{m,n} \Im \{ [\int_0^L \tau_\nu(s) [\bar{Y}^m \cdot Y^n](s) \int_0^s \tau_\nu(t) [\bar{Y}^n \cdot Y^m](t) dt \}.$$

But additionally, the symbol of the commutator involves the third transvectant P_3 of §4.3, and the P_3 of any two monomials of degree 3 is a constant in z.

We observe that there is no term of order $|z|^2$ since the Poisson bracket of two homogeneous polynomials of degree 3 has degree 4 and the P_3-transvectant has degree zero. This proves Lemma 6.4 and also:

LEMMA 6.6. *On a Zoll surface, the coefficient of $|z|^4$ or 1 in the commutator term* (45) *is a sum of universal constants times*

$$\frac{1}{L} \{ \int_0^L \tau_\nu(s) \bar{Y}^m Y^n(s) [\int_0^s \tau_\nu(t) \bar{Y}^n Y^m](t) dt] ds$$

$$- \int_o^L \tau_\nu(s) \bar{Y}^n Y^m(s) [\int_0^s \tau_\nu(t) \bar{Y}^m Y^n(t) dt] ds \}$$

$$= 2 \frac{1}{L} \Im \int_0^L \tau_\nu(s) \bar{Y}^m Y^n(s) [\int_0^s \tau_\nu(t) \bar{Y}^n Y^m](t) dt] ds.$$

REMARK 6.7. *There are many 'off-diagonal' terms in the commutator corresponding to $[z^m \bar{z}^n, z^p \bar{z}^q]$ which are not a power of $|z|^2$. These obviously produce terms of the form*

$$\{ [\int_0^L \tau_\nu(s) [\bar{Y}^m \cdot Y^n](s) \int_0^s \tau_\nu(t) [\bar{Y}^q \cdot Y^p](t) dt \}.$$

On a Zoll surface the complete sum of the off-diagonal terms must vanish.

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6.3.2. *Diagonal terms of* $\mathcal{D}_0|_0$. To complete the calculation of (44), we need to find the symbol of the D_s-weight 0 part $\mathcal{D}_0|_0$ of the remaining term of $\mathcal{D}_0^{\frac{1}{2}}$ in (48). We make the same linear substitution and eliminate any D_s appearing all the way to the right. We also invert the relation

$$\mu(\mathcal{A}^*)^{-1} D_s \mu(\mathcal{A}^*) = D_s - \frac{1}{2}(\partial_x^2 + \tau x^2)$$

to get

$$\mu(\mathcal{A}^*) D_s \mu(\mathcal{A}^*)^{-1} = D_s - \frac{1}{2}\mu(\mathcal{A}^*)(\partial_x^2 + \tau x^2)\mu(\mathcal{A}^*)^{-1}$$

and transform the complete symbol of quadratic term by the symplectic substitution. The result is that

LEMMA 6.8. $\mathcal{D}_0|_0(s, z, \bar{z})$ *equals*

(i) $\quad C_1 \tau_{\nu\nu}[\bar{Y}z + Y\bar{z}]^4 + C_3 \tau_s [\bar{Y}z + Y\bar{z}]^2$

(ii) $\quad + C_2 \tau [\bar{Y}z + Y\bar{z}]^2 \#([\bar{\dot{Y}}z + \dot{Y}\bar{z}]^2 + \tau[\bar{Y}z + Y\bar{z}]^2))$

(iii) $\quad + \{[\bar{\dot{Y}}z + \dot{Y}\bar{z}]^2 - \tau[\bar{Y}\cdot z + Y\bar{z}]^2\} \# \{[\bar{\dot{Y}}z + \dot{Y}\bar{z}]^2 - \tau[\bar{Y}z + Y\bar{z}]^2\}$

(iv) $\quad -2\partial_s([\bar{\dot{Y}}z + \dot{Y}\bar{z}]^2 - \tau[\bar{Y}z + Y\bar{z}]^2)$

(v) $\quad + C_4 \tau(\bar{Y}z + Y\bar{z}) \# (\bar{\dot{Y}}z + \dot{Y}\bar{z}) + C_5 \tau.$

Our concern is with the diagonal part of the complete symbol, that is, with the terms involving $|z|^4, |z|^2, |z|^0$, and more precisely with their integrals over γ. The # product produces a finite sum terms of decreasing degree corresponding to the higher transvectants.

The diagonal part of the first term of (i) is homogeneous of degree $|z|^4$ and its average over γ equals

$$(Const.)|z|^4 \cdot \frac{1}{L}\int_0^L \tau_{\nu\nu}|Y|^4 ds.$$

It is the "d_j" term in the formula of Theorem 1 and is clearly only a coefficient of $|z|^4$; this explains why the term does not appear as a coefficient of $|z|^0$. The integral of the diagonal part of the second term of (i) vanishes,

$$\int_0^L \tau_s |Y|^2 = 0,$$

as can be seen from the Jacobi equation, which implies:

$$[\bar{Y}(Y')'' + \tau_s|Y|^2 + \tau Y'\bar{Y}] = 0;$$

integrating over γ and integrating the first term by parts twice kills the outer terms and hence the inner one.

Terms (ii) and (iii) are similar and possibly combine. Term (iii) is a #-square, as is one of the two terms of (ii).

The diagonal part of the # product in (ii) contributes only P_0 and P_2 terms, of degrees $|z|^4$ and $|z|^0$ respectively. The $|z|^4$ coefficient is that of

$$\tau^2[\bar{Y}z + Y\bar{z}]^4 + \tau[\bar{Y}z + Y\bar{z}]^2[\bar{\dot{Y}}z + \dot{Y}\bar{z}]^2 = (\tau^2|Y|^4 + \tau|Y\dot{Y}|^2)|z|^4 + \cdots,$$

where the $\cdots$ terms are homogeneous of degree 4 but do not contain a term of type $|z|^4$. The integral over γ of the possible P_1-term of type $|z|^2$ vanishes: it is a multiple of the Poisson bracket

$$P_1([\bar{Y}z + Y\bar{z}]^2, \tau[\bar{Y}z + Y\bar{z}]^2))$$

which simplifies to a term of the form

$$\tau[\bar{Y}^2\dot{Y}^2 - Y^2\dot{\bar{Y}}^2] = \tau(\bar{Y}\dot{Y} - Y\dot{\bar{Y}})(\bar{Y}\dot{Y} + Y\dot{\bar{Y}}) = C\tau\frac{d}{ds}|Y|^2$$

by the symplectic normalization of the Jacobi eigenfield. As mentioned above, its integral vanishes. The P_0 term is obtained by applying the square of the bi-differential operator

$$\sum_j (\partial_{z_j}\partial_{\bar{w}_j} - \partial_{\bar{z}_j}\partial_{w_j})f(z)g(w)$$

to the expression with f on the left and g on the right and setting $z = w$.

The term (iii) is a homogeneous #-square, hence its diagonal part contains only a product P_0-term of degree $|z|^4$ and a P_2-term of degree 0, namely (for j=0,2) the diagonal part of

$$P_j[z^2\dot{\bar{Y}}^2 + 2|z|^2|\dot{Y}|^2 + \bar{z}^2\dot{Y}^2 - \tau(z^2\bar{Y}^2 + 2|z|^2|Y|^2 + \bar{z}^2Y^2),$$

$$z^2\dot{\bar{Y}}^2 + 2|z|^2|\dot{Y}|^2 + \bar{z}^2\dot{Y}^2 - \tau(z^2\bar{Y}^2 + 2|z|^2|Y|^2 + \bar{z}^2Y^2)]$$

whose average over γ has the form for $j = 2, 0$

$$\int_0^L [a_j|\dot{Y}|^4 + b_{1j}\tau 2\Re(\dot{\bar{Y}}^2Y^2) + 2b_{2j}\tau|\dot{Y}Y|^2 + c_j\tau^2|Y|^4]ds$$

where

$$a_j = c_j = 2P_j(z^2, \bar{z}^2) + 2P_j(|z|^2, |z|^2), \quad b_{1j} = -2P_j(z^2, \bar{z}^2) = b_{2j}$$

Note here than P_j is symmetric if j is even and that $P_2(z^2, \bar{z}^2) = -2P_2(|z|^2, |z|^2)$. Also

$$2\Re(\dot{\bar{Y}}^2Y^2) + 2|\dot{Y}Y|^2 = (\dot{Y}\bar{Y} + \overline{\dot{Y}Y})^2.$$

In Lemma 7.2 we show that

$$\int_\gamma |\dot{y}|^4 ds = 2\int \tau|Y\dot{Y}|^2 ds + \Re\int_\gamma \tau(\dot{Y}\bar{Y})^2 ds.$$

The diagonal term of (iv) has vanishing integral since it is a total derivative. Finally, we the first term of (v) obviously has no diagonal part while obviously the second term contributes the zeroth order term

$$C\int_\gamma \tau ds.$$

Adding the terms of Lemma 6.6 and Lemma 6.8 completes the analysis of the Birkhoff normal form coefficient $f_0(I)$ in the Zoll case. It must vanish in the maximally degenerate case.

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6.4. Off-diagonal terms. In the MDL Zoll case, existence of the normal form implies that the off-diagonal terms must vanish and triviality of the normal form implies that the diagonal terms vanish. Above we emphasized the diagonal terms. We now briefly consider the off-diagonal ones.

From the commutator terms (50) we obtain off-diagonal terms

(51)

$$\sum_{m+n=3,p+q=3} C'_{m,n,p,q}\{[\int_0^L \tau_\nu(s)[\bar{Y}^m \cdot Y^n](s) \int_0^s \tau_\nu(t)[\bar{Y}^p \cdot Y^q](t)dt\}[z^m\bar{z}^n, z^p\bar{z}^q],$$

where $[z^m\bar{z}^n, z^p\bar{z}^q] = \{z^m\bar{z}^n, z^p\bar{z}^q\} + C_3P_3(z^m\bar{z}^n, z^p\bar{z}^q)$. Thus we obtain the same geometric invariants as in the diagonal case, but with different coefficients determined by transvectants of monomials. The Poisson bracket gives all possible monomials of degree 4 and P_3 gives the two mononomials of degree 1.

Lemma 6.8 expresses $\mathcal{D}_0|_0(s, z, \bar{z})$ as a sum of compositions involving P_4, P_3, P_2, P_1, P_0 where P_0 is simply multiplication. We then obtain a sum of monomials of degrees ≤ 4. Adding to the commutator terms gives coefficients of monomials $z^a\bar{z}^b$ with $a + b \leq 4$ and the coefficient must vanish for every monomial. We worked out the monomials $1, |z|^2, |z|^4$ in detail because they are the ones that arise in the Birkhoff normal form construction in the non-degenerate case. But the vanishing of the off-diagonal monomial coefficients is just as informative as the vanishing of the diagonal ones. Since the transvectant coefficients differ, it is likely that by taking linear combinations of all of the invariants defined as coefficients of monomials, we can simplify the condition of Theorem 1.

7. Final Remarks

There are many open problems regarding Zoll Laplacians, some of which might not be difficult to answer. As mentioned before, they are tests of the known techniques in inverse spectral theory. We close with some observations and speculations as well as with some further identities which simplify Theorem 1.

7.1. Analysis of $p_1(q)$. We observe that each the integrals over closed geodesics in the expression for $p_1(q)$ in Theorem 1 defines a function on $S^*_gS^2$. To see this, we observe that (x, ξ) determines the closed geodesic $\gamma_{x,\xi}(t) = \pi G^t(x, \xi)$ where G^t is the geodesic flow. The basis of Jacobi fields y_1, y_2 with Wronskian matrix (12) equal to the identity at $t = 0$ is then determined uniquely by (x, ξ). The various terms above are integrals over $\gamma_{x,\xi}$ and thus each term is a function of (x, ξ). Also $\nu = J\dot{\gamma}$ is defined by (x, ξ) and the unique complex structure J of S^2.

Similarly, each term of the integrand is a function of $(x, \xi, t) \in S^*_gS^2 \times S^1$. The entire integrand for the coefficient c_{2j} of p_1 defines a function $F_j(x, \xi, t)$ on $S^*_gS^2 \times S^1$ depending on the index j. In the maximally degenerate case, or more generally when $p_1 = 0$, $F_{2j} = \frac{\partial}{\partial t} f_{2j}$ for some smooth function f_{2j}. Equivalently, if Ξ generates the geodesic flow, then $F_{2j} = \Xi f_{2j}$. If we expand F as a Fourier series in the t variable, we have

$$F(x, \xi, t) = \sum_{n\in\mathbb{Z}.n\neq 0} \hat{F}(x, \xi, n)e^{int}, \quad f(x, \xi, t) = \sum_{n\in\mathbb{Z}.n\neq 0} \frac{\hat{F}(x, \xi, n)}{in} e^{int}.$$

But F is constructed in a universal way from the Zoll metric.

This condition is satisfied by the standard metric. An obvious question is whether $\sigma_{A_0} = 0$ for any non-standard Zoll metric g. In fact, it is not even obvious whether there may exist a deformation of the standard metric g_0 through Zoll

metrics for which $\sigma_{A_0}(g_t) = 0$ for $t \in [0, \epsilon]$ for some $\epsilon > 0$. It is hoped that Theorem 1 could provide some information on this question. In fact it is not even clear that there exist any Zoll surfaces for which $\sigma_{A_0}(g) = 0$ although it was found in [**Z1**] that no Zoll surfaces of revolution have this property.

In the case of potential perturbations $\Delta_0 + V$ on the standard S^2 the analogous symbol is $\int_\gamma V ds$ and it is not hard to show that only $V = 0$ is maximally degenerate. The proof uses the explict formula for the normal form of the operator. This suggests that we must rely on the expression in Theorem 1 in the metric case.

Of course, in the MDL case all of the terms of the Birkhoff normal form expansion vanish, and the Zoll Laplacian has the form $\mathcal{R}(\mathcal{R}+1)+\mathcal{S}$ where $\mathcal{S}$ is smoothing and is a function of $\mathcal{R}$. In [**Z1**] the trace of $\mathcal{S}$ is determined and in principal one could determine $Tr\mathcal{S}^n$ for any n using the heat kernel expansion for

$$\begin{aligned}\exp -t(\mathcal{R}(\mathcal{R}+1)+\mathcal{S}) &= \exp(-t\mathcal{S})\exp(-t\mathcal{R}(\mathcal{R}+1)) \\ &= \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} Tr\mathcal{S}^n \exp(-t\Delta_0) \\ &\sim Tre^{-t\Delta_0} + \sum_{n=1}^{\infty} \frac{(-t)^n}{n!} \sum_{m=0}^{\infty} \frac{(-t)^m}{m!} Tr\mathcal{S}^n \Delta_0^m, \quad (t \to 0),\end{aligned}$$

where $\Delta_0 = \mathcal{R}(\mathcal{R}+1)$ has the same eigenvalues and multiplicities as the standard Laplacian. One might try to determine $\mathcal{S}(k)$ completely from these traces using the heat kernel expansion, or prove that no such $\mathcal{S}(k)$ can exist. However, there are many terms producing a given order of t^M.

One might also think in terms of the infinite dimensional moduli space $\mathcal{Z}$ of Zoll metrics on S^2 [**G3**]. Its tangent space at a Zoll metric g consists of the kernel of the geodesic Radon transform of g on $C^\infty(S^2)$. In the case of the standard metric, the kernel consists of the odd functions. The function $F(x, \xi, t; g)$ is constructed in a universal way from the 4-jet g, Dg, D^2g, D^3g, D^4g of the metric on the moduli space of Zoll metrics. Hence the terms of $p_1(g)$ define 'natural' maps from $\mathcal{Z} \to C^\infty(S^*_g M)$ with equivariance under G^t, so $p_1(g)$ is a natural function on $G(M, g)$. Of course, the symbol of A_{-1} is of this kind. There might exist a geometric functional on $\mathcal{Z}$ which is critical exactly at MDL metrics. But since it is a spectral condition, the functional would most likely be a spectral one.

7.2. Balancing issues. In [**Z3**] this question was approached via the spectral projections kernels $\Pi_k(x, y)$ for the eigenvalue clusters rather than through Gaussian beams and normal forms. In the maximally degenerate case, the eigenmap embeddings $y \to \Pi_k(\cdot, y) : S^2 \to \mathcal{H}_k$ are almost isometric up to order $k^{-\infty}$. Here $\mathcal{H}_k$ is the Hilbert space of eigenfunctions of Δ_g for the kth cluster (in the MDL case); see §5.1 for background. The metric g would have to be the standard one if the maps were exactly isometric. In the Gaussian beam setting we instead have the maps

$$H_k : G(S^2, g) \simeq S^2 \to \mathcal{H}_k, \quad H_k(\gamma) = \varphi_k^\gamma,$$

although to be precise φ_k^γ is defined only up to a constant (depending on a choice of basepoint for γ), and it would be better to define the map to the projective space of $\mathcal{H}_k$. Again, the map H_k is almost isometric in the MDL case, as follows by combining the formula for Π_k in §5.1 with the results of [**Z3**].

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The article preceded [**Z3**] predated the modern era of balanced Kähler metrics and Bergman metrics but is somewhat related in spirit. There is a well-known analogy between Zoll surfaces and positive line bundles over Kähler surfaces in which the unit tangent bundle of the Zoll surface is parallel to the Hermitian metric unit bundle. In both cases the unit bundle is an S^1-bundle. Indeed, it is more than an analogy since the unit tangent bundle is a circle bundle over the space $G(S^2, g)$ of geodesics of g and is the unit bundle for a Hermitian metric of positive $(1,1)$ curvature on the holomorphic line $T\mathbb{CP}^1$ over $G(S^2, g)$. It is not clear what if any implications maximal degeneracy of Δ_g has for the Szegö kernel of this line bundle or for its $\bar\partial$-Laplacian. For instance, the spectral projections kernel Π_k of a MDL is almost constant on the diagonal (modulo a term of order $k^{-\infty}$). Is the same true for the associated Szegö kernel of $H^0(\mathbb{CP}^1, (T\mathbb{CP}^1)^{\otimes k})$?

7.3. Relations among terms. We note some relations between the integrals in Theorem 1. They allow for some simplification of the expression for $p_1(q)$ and suggest that other simplifications might exist. They also help in comparing Theorem 1 with the formulae in [**Z1**, **Z3**] but for the sake of brevity we do not make a detailed comparison.

LEMMA 7.1. *For any solution of the Jacobi equation of any Zoll surface,*

$$\int \tau y^2 \dot y^2 ds = \frac{1}{3}\int (\dot y)^4 ds.$$

To prove this we multiply the Jacobi equation by $\dot y^2 y$ and use that

$$\int \dot y^2 y \ddot y ds = -\int \dot y \frac{d}{ds}(y\dot y^2) ds = -\int (2\dot y^2 y\ddot y - \dot y^4) d.$$

Jacobi's equation implies that

$$-\int \dot y^2 y\ddot y ds = \int \tau y^2 \dot y^2 ds.$$

Combining the formulae concludes the proof.

A variant that applies directly to Theorem 1 is the following.

LEMMA 7.2. *For an Zoll surface and close geodesic*

$$\Im \int_\gamma \tau(\dot y\bar y)^2 ds = 0, \quad \int_\gamma |\dot y|^4 ds - 2\int \tau |y\dot y|^2 ds = \Re \int_\gamma \tau(\dot y \bar y)^2 ds.$$

This allows us to remove the third term (the b_2 term) and with universal changes in the coefficients of the first two terms.

PROOF. Consider the term,

$$\int \tau |y\dot y|^2 ds = \int \tau y\bar y \dot y \overline{\dot y} ds.$$

Multiply the Jacobi equation for y by $\bar y \dot y \overline{\dot y}$. Jacobi's equation implies that

$$\int \tau |y\dot y|^2 ds = -\int \ddot y \bar y \dot y \overline{\dot y} ds.$$

We also have

$$\begin{aligned} -\int \ddot{y}\bar{y}\dot{y}\dot{\bar{y}}ds &= \int \dot{y}\tfrac{d}{ds}(\bar{y}\dot{y}\dot{\bar{y}})ds \\ &= \int \dot{y}(\tfrac{d}{ds}(\bar{y})\dot{y}\dot{\bar{y}})ds + \int \dot{y}(\bar{y}\tfrac{d}{ds}\dot{y})\dot{\bar{y}})ds + \int \dot{y}(\bar{y}\dot{y}\tfrac{d}{ds}\dot{\bar{y}})ds \\ &= \int \dot{y}^2\dot{\bar{y}}^2 ds - \int \dot{y}(\bar{y}\tau y)\dot{\bar{y}})ds - \int \dot{y}(\bar{y}\dot{y}\tau\bar{y})ds. \end{aligned}$$

Hence

$$2\int \tau|y\dot{y}|^2 ds = \int |\dot{y}|^4 ds - \int \tau(\dot{y}\bar{y})^2 ds.$$

All the terms are real except the last one, so its imaginary part is zero.

□

We may also simplify the "commutator term" of Theorem 1. A real orthogonal Jacobi field $Y = y\nu$ along γ defines a variation $\gamma_r(t)$ of $\gamma(t)$ with variational vector field Y. We then have a 1-parameter family of Jacobi fields $Y_r(t)$ on $\gamma_r(t)$ and can differentiate with respect to r. We denote the derivative of y_r by y_ν (possibly not good notation). For any Jacobi field we get the equation $y_\nu'' + \tau_\nu y^2 + \tau y_\nu = 0$ for this varation. Multiply by a section Jacobi field y_2 to get $y_\nu'' y_2 + \tau_\nu y^2 y_2 + \tau y_\nu y_2 = 0$ Therefore

$$\tau_\nu y^2 y_2 = -(y_\nu'' y_2 + \tau y_\nu y_2).$$

It follows that

$$\begin{aligned} -\int_0^s \tau_\nu(t)\bar{Y}^n Y^m(t)dt &= \int_0^s (y_\nu'' y_2 + \tau y_\nu y_2))dt \\ &= y_\nu' y_2|_0^s - \int_0^s (y_\nu' y_2' + \tau y_\nu y_2) \\ &= y_\nu' y_2|_0^s - (y_\nu y_2')|_0^s \\ &= Y_\nu'(s)\overline{Y}(s) - Y_\nu(s)\overline{Y}'(s) - Y_\nu'(0) + iY_\nu(0). \end{aligned}$$

Since $Y = y_1 + iy_2, \overline{Y} = y_1 - iy_2$ if $y_2 = \overline{Y}$ we have $y_2(0) = 1, y_2'(0) = -i$. Since $Y(0) = 1, Y'(0) = i$ for all γ, the variations of these quantities vanish and the last two terms are zero. Therefore,

$$\begin{aligned} &\Im\{\textstyle\int_0^{2\pi} \tau_\nu(s)\bar{Y}^m Y^n(s)[\int_0^s \tau_\nu(t)\bar{Y}^n Y^m](t)dt]ds\} \\ &= \Im\{\textstyle\int_0^{2\pi} \tau_\nu(s)\bar{Y}^m Y^n(s)[Y_\nu'(s)\overline{Y}(s) - Y_\nu(s)\overline{Y}'(s)]ds\} \\ &= \textstyle\int_0^{2\pi} \tau_\nu(s)\Im\{\bar{Y}^m Y^n(s)[Y_\nu'(s)\overline{Y}(s) - Y_\nu(s)\overline{Y}'(s)]\}ds. \end{aligned}$$

For instance, if $m = 2, n = 1$ the "commutator term" is equal to

$$\int_0^{2\pi} \tau_\nu(s)\Im\{\bar{[}Y(s)Y_\nu'(s)\overline{Y}^3(s) - Y(s)Y_\nu(s)\overline{Y(s)}^2\overline{Y}'(s)]\}ds$$

Also, the Wronskian condition

$$Y(s)\overline{Y}'(s) - Y'(s)\overline{Y}(s) = i$$

holds for all γ and therefore its variation vanishes. Thus,

$$Y_\nu(s)\overline{Y}'(s) - Y_\nu'(s)\overline{Y}(s) + Y(s)\overline{Y}_\nu'(s) - Y'(s)\overline{Y}_\nu(s) = 2\Im(Y_\nu(s)\overline{Y}'(s) - Y_\nu'(s)\overline{Y}(s)) = 0.$$

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Thus,

$$\int_0^{2\pi} \tau_\nu(s)\Im\{\bar{Y}^m Y^n(s)[Y'_\nu(s)\overline{Y}(s) - Y_\nu(s)\overline{Y}'(s)]\}ds$$
$$= \int_0^{2\pi} \tau_\nu(s)\Im\{\bar{Y}^m Y^n(s)\}[Y'_\nu(s)\overline{Y}(s) - Y_\nu(s)\overline{Y}'(s)]ds.$$

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