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Embedded eigenvalues, localization and asymptotics of quantum field models: a functional integral approach

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Abstract

By means of functional integrals, a Hamiltonian of a system of a charged particle coupled to a quantized radiation field is investigated, it is the so called Pauli–Fierz model in nonrelativistic quantum electrodynamics. Embedded eigenvalues of the Hamiltonian with a singular external potential are studied and their multiplicities are estimated. The localization of a charge density of eigenvectors is considered. A partial trace of the semigroup generated by the Hamiltonian is defined and its classical limit, $\hbar \rightarrow 0$, is discussed. Finally a nonrelativistic limit, $c \rightarrow \infty$, is considered.

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1. Introduction and main results

We investigate a system of a charged particle minimally coupled with a quantized radiation field, which is the so called Pauli–Fierz model in nonrelativistic QED [23]. The quantized radiation field is massless and an ultraviolet cutoff is imposed. The Pauli–Fierz model has been an important model in, e.g., quantum optics, atomic physics, etc, see [29]. It is also well known that the Pauli–Fierz model successfully describes an interaction between low energy electrons and photons. In particular it gave an interpretation of the Lamb shift [31].

Let \mathcal{F}_{PF} be the symmetric Fock space over $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$,

$$\mathcal{F}_{\text{PF}} = \bigoplus_{n=0}^{\infty} \otimes_s^n (L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$$

where \otimes_s^n denotes the n -fold symmetric tensor product with $\otimes_s^0(\cdot \cdot \cdot) = \mathbb{C}$. We denote the two component annihilation and creation operator in \mathcal{F}_{PF} by $a^\dagger(k, j)$ and $a(k, j)$, $j = 1, 2$,

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respectively, which satisfy the canonical commutation relations

$$\begin{aligned} [a(k, j), a^\dagger(k', j')] &= \delta_{jj'}(k - k') \\ [a^\dagger(k, j), a^\dagger(k', j')] &= [a(k, j), a(k', j')] = 0 \quad k, k' \in \mathbb{R}^3. \end{aligned}$$

For each $x \in \mathbb{R}^3$, a quantized radiation field is defined by

$$A_{\text{PF}}(x) = \frac{1}{\sqrt{2}} \sum_{j=1,2} \int \frac{\sqrt{c\hbar} \vec{e}_j(k)}{\sqrt{(2\pi)^3 \omega(k)}} \{a^\dagger(k, j) e^{-ikx} \hat{\rho}(-k) + a(k, j) e^{ikx} \hat{\rho}(k)\} dk$$

where ρ describes a charge density of a particle, and $\hat{\rho}$ its Fourier transform. Here, $\omega(k) = |k|$ the dispersion relation, c the velocity of the light, \hbar the Planck constant divided by 2π and $\vec{e}_j(k) = (e_j^1(k), e_j^2(k), e_j^3(k))$ polarization vectors forming the right-hand dreibein in \mathbb{R}^3 , i.e.

$$\vec{e}_j(k) \cdot \vec{e}_{j'}(k) = \delta_{jj'} \quad \vec{e}_j(k) \cdot k = 0 \quad \vec{e}_1(k) \times \vec{e}_2(k) = k/|k|.$$

The free Hamiltonian is defined by

$$H_{\text{b}} = \sum_{j=1,2} \int \omega(k) a^\dagger(k, j) a(k, j) dk.$$

Under these preparations the Pauli–Fierz Hamiltonian H_{PF} is defined as an operator acting on the Hilbert space

$$\mathcal{H}_{\text{PF}} = L^2(\mathbb{R}^d) \otimes \mathcal{F}_{\text{PF}}$$

by

$$H_{\text{PF}} := \frac{1}{2} \left(p \otimes 1 - \frac{e}{c} A_{\text{PF}}(x) \right)^2 + \hbar c 1 \otimes H_{\text{b}} + V \otimes 1$$

where $p = -i\hbar \nabla_x$ denotes the momentum operator canonically conjugate to the position operator x , V an external potential, e the charge of a particle (a coupling constant).

Here we review a short history of H_{PF} from a mathematical point of view. The *dipole approximation* of H_{PF} , say $H_{\text{PF}}^{\text{dip}}$, is defined by H_{PF} with $A_{\text{PF}}(x)$ replaced by $A_{\text{PF}}(0)$, i.e.

$$H_{\text{PF}}^{\text{dip}} := \frac{1}{2} \left(p \otimes 1 - 1 \otimes \frac{e}{c} A_{\text{PF}}(0) \right)^2 + \hbar c 1 \otimes H_{\text{f}} + V \otimes 1. \quad (1.1)$$

The dipole approximation corresponds to neglecting collisions between the particle and photons. Several papers have been devoted to the study of (1.1). In particular Arai [1, 2] diagonalized (1.1) with some potentials and its spectral properties were investigated.

A lattice approximation can give more precise spectral information about $H_{\text{PF}}^{\text{dip}}$. Take a momentum lattice $\mathbb{L} \subset \mathbb{R}^d$ of width $1/a$ with the finite volume $(2L)^d$, and the number of lattice points is $N = (2aL + 1)^d$. The l th lattice is denoted by Γ_l , $l = 1, \dots, N$. A momentum lattice approximation of (1.1), say $H_{\text{PF}}^{\text{Lattice}}$, is defined by $\hat{\rho}$, ω , and e_j^μ replaced by $\sum_{l=1}^N \hat{\rho}(l_c) \chi_{\Gamma_l}$, $\sum_{l=1}^N \omega(l_c) \chi_{\Gamma_l}$ and $\sum_{l=1}^N e_j^\mu(l_c) \chi_{\Gamma_l}$, respectively, where χ_{Γ_l} denotes the characteristic function of Γ_l and l_c the point of the centre of Γ_l . It is seen that

$$\mathcal{H}_{\text{PF}} \cong L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^{(d-1)N})$$

and

$$H_{\text{PF}}^{\text{Lattice}} \cong \frac{1}{2} \sum_{\mu=1}^d \left(p_\mu - \sum_{l=1}^N v_l^\mu \cdot q_l \right)^2 + \sum_{l=1}^N \left(\frac{p_l^2}{2} + \frac{1}{2} \omega(l_c) q_l^2 \right) - (d-1) \sum_{l=1}^N \sqrt{\omega(l_c)} + V(x) \quad (1.2)$$

where \simeq denotes unitary equivalence, $\{q_l, p_l\}_{l=1}^N$ the canonical pairs of $L^2(\mathbb{R}^{(d-1)N})$, v_l^μ , $\mu = 1, \dots, d$, are some vectors in \mathbb{R}^{d-1} . Moreover it was established that for $z \in \mathbb{C} \setminus \mathbb{R}$

$$\lim_{L \rightarrow \infty} \lim_{a \rightarrow \infty} (H_{\text{PF}}^{\text{Lattice}} - z)^{-1} = (H_{\text{PF}}^{\text{dip}} - z)^{-1} \tag{1.3}$$

in the operator norm. See [19, appendix] for details. Equation (1.2) has been exactly solved by Ford, Lewis and O’Connell [10, 11]. Certain spectral properties of (1.2) can be transmitted to those of (1.1). In fact the exact ground state energy and an effective mass of $H_{\text{PF}}^{\text{dip}}$ with $V = 0$ has been calculated through (1.2) and (1.3).

The next question which we must consider is the full Pauli–Fierz Hamiltonian. It must be noted that no dipole approximation makes the problem extremely serious. Over the past few years, by using quite different ways from the dipole approximation case, a considerable number of studies have been done in, e.g., [4–6, 13].

There are three kinds of problems studied in this paper.

- (I) Embedded eigenvalues of H_{PF} with a *singular* external potential V , and their multiplicities.
- (II) Localization of a charge density of eigenvectors.
- (III) Classical and nonrelativistic limits of H_{PF} .

The first consideration is (I): in the study of the spectrum of H_{PF} , particular attention is paid to the questions of whether the ground state of H_{PF} exists or not, and of its multiplicity. The decoupled Hamiltonian, H_d , is defined by H_{PF} with e replaced by zero:

$$H_d := H_p \otimes 1 + 1 \otimes H_b$$

where H_p is the particle Hamiltonian:

$$H_p := \frac{1}{2} p^2 + V.$$

It is known that²

$$\sigma(H_b) = [0, \infty).$$

Thus in the case of $\sigma(H_p) = \{E_j(0)\}_{j=0}^N \cup [\Sigma, \infty)$, it follows that

$$\sigma(H_d) = [E_0(0), \infty)$$

and

$$\sigma_p(H_d) = \{E_j(0)\}_{j=0}^N.$$

Hence our analysis is reduced to a perturbation problem of embedded eigenvalues $E_j(0)$ ’s in the continuum. Bach–Fröhlich–Sigel [4–6] proved the existence of a ground state of H_{PF} and an instability of embedded eigenvalues, i.e. resonances, for weak couplings under some suitable conditions. Griesemer–Lieb–Loss [13] proved the existence of a ground state of H_{PF} for arbitrary couplings. Hiroshima [15] showed the uniqueness of the ground state for some smooth external potentials for arbitrary couplings. It is noteworthy that resonances and the uniqueness of the ground state are proved for some smooth external potential, e.g. it is relatively bounded with respect to the Laplacian. In this paper, taking a singular external potential, we construct H_{PF} such that

- (I-i) H_{PF} has embedded eigenvalues $\{E_j\}_{j=1}^M$
- (I-ii) $E_j \rightarrow E_j(0)$ as $e \rightarrow 0$.

² We denote by $\sigma(T)$ (respectively $\sigma_p(T), \sigma_{\text{disc}}(T), \sigma_{\text{ess}}(T)$) the spectrum of T (respectively the point spectrum of T , the discrete spectrum of T , the essential spectrum of T).

In particular (I-ii) gives an example such that an embedded eigenvalue of H_d does *not* move to resonances after adding a perturbation. We prove that there exists a class of singular potentials $\mathcal{P}_{\text{sing}}$ and a positive constant $e_g(V)$ such that

Theorem 1.1. *Let $V \in \mathcal{P}_{\text{sing}}$ and $|e| \leq e_g(V)$. Then there exists embedded eigenvalues E_j 's in the continuum and $\lim_{e \rightarrow 0} E_j = E_j(0)$.*

One of the examples of singular potentials is of the form

$$V_\nu(x) := \frac{\nu}{|x - \partial\Omega|^3} + |x|^2.$$

Here Ω is an open set in \mathbb{R}^3 , $\partial\Omega$ its boundary and $\nu > 0$ a positive constant. V_ν divides \mathbb{R}^3 into its connected components with boundary $\partial\Omega$. Then H_{PF} acts on vectors vanishing on $\partial\Omega$. This is a mathematical reason behind such a result that H_{PF} is reduced by $L^2(D_j) \otimes \mathcal{F}$ with some connected components D_j 's. This is proved through a functional integral technique. We then show that $H_{\text{PF}} \upharpoonright_{L^2(D_j) \otimes \mathcal{F}}$ has a unique ground state and its corresponding eigenvalue, the ground state energy, is embedded in the continuum of H_{PF} .

The second consideration is (II): in quantum mechanics, an exponential decay of the charge density of an eigenvector is standard folklore. In fact such an exponential decay was shown by many authors, e.g. [26], on quantum mechanics grounds. Our interest is whether an exponential decay is a stable property or not, when the particle interacts with quantized radiation fields. Regarding H_{PF} as the set of \mathcal{F}_{PF} -valued L^2 functions, $L^2(\mathbb{R}^d; \mathcal{F}_{\text{PF}})$, Ψ_p becomes an \mathcal{F}_{PF} -valued L^2 function. The question now arises: does $\|\Psi_p(x)\|_{\mathcal{F}_{\text{PF}}}$ exponentially decay in x ? It depends on external potentials. We specify classes $V(m)$, $m = 0, 1, 2, \dots$, of external potentials.

Theorem 1.2. *Let Ψ_p be an arbitrary eigenvector of H_{PF} . Suppose $V \in V(m)$. Then*

$$\|\Psi_p(x)\|_{\mathcal{F}_{\text{PF}}} \leq D e^{-\delta|x|^{m+1}} \quad a.e. x \in \mathbb{R}^3$$

with some constants D and δ .

Although in [5] and [13] such an exponential decay is derived, it is in quite a different way from ours. Moreover our result is almost everywhere pointwise.

We have some comments on theorem 1.2. In [19] we proved that for sufficiently *large* $|e|$ a ground state of H_{PF} appears even if H_p has no ground states, e.g. H_p has a sufficiently shallow nonpositive external potential. Our next interest is to investigate an exponential decay of the charge density of a ground state appearing in the enhanced binding. Unfortunately we are unable to discuss this question, so that it must be left aside and is considered elsewhere.

The final consideration is (III): there are two reasons for investigating asymptotics of H_{PF} ; it is important to see how H_{PF} contains a successful quantum mechanical theory as the limiting case $c \rightarrow \infty$ and classical mechanical theory as $\hbar \rightarrow 0$; moreover, practically it is useful to replace H_{PF} by simpler quantum or classical models together with some corrections.

We discuss a nonrelativistic limit of H_{PF} in the sense of semigroups.

Theorem 1.3. *Let P_Ω be the projection onto a one-dimensional subspace spanned by the vacuum of \mathcal{F}_{PF} . Then*

$$s - \lim_{c \rightarrow \infty} e^{-tH_{\text{PF}}} = e^{-tH_p} \otimes P_\Omega.$$

In the classical limit, since H_{PF} has a spectral continuum, we have to modify a usual definition of trace of $e^{-tH_{\text{PF}}}$. For $\Psi \in \mathcal{F}$, the bilinear form

$$B(f, g) := (f \otimes \Psi, e^{-tH_{\text{PF}}} g \otimes \Psi)_{\mathcal{H}} \quad f, g \in L^2(\mathbb{R}^d)$$

defines a bounded operator B on $L^2(\mathbb{R}^d)$ such that³ $B(f, g) = (f, Bg)_{L^2(\mathbb{R}^d)}$. Then we can define a partial trace of $e^{-tH_{\text{PF}}}$ by

$$\text{Tr}_\Psi(e^{-tH_{\text{PF}}}) := \text{Tr}(B)$$

under some conditions. Let

$$\text{Tr}_{\text{cl}}\left(e^{-t(p^2/2+V(x))}\right) := (2\pi\hbar)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-t(p^2/2+V(x))} dp dx.$$

Then we show that

Theorem 1.4. *Suppose $e^{-tV} \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and V is continuous. Then*

$$\lim_{\hbar \rightarrow 0} \text{Tr}_\Psi(e^{-tH_{\text{PF}}}) / \text{Tr}_{\text{cl}}\left(e^{-t(p^2/2+V(x))}\right) = \|\Psi\|_{\mathcal{F}_{\text{PF}}}^2.$$

This paper is organized as follows: in section 2 taking a Schrödinger representation instead of the Fock representation mentioned above, we define a Hamiltonian H on some L^2 space, which is unitarily equivalent to H_{PF} , and give a brief review of a functional integral representation of e^{-tH} . In section 3 we consider H with a singular external potential, and study embedded eigenvalues. Section 4 is devoted to considering localization of a charge density of eigenvectors. In section 5 we investigate both classical and nonrelativistic limits. Theorems 1.1–1.4 shall be stated in theorems 3.6, 4.4, 5.2 and 5.10 respectively.

2. Quantum field models

2.1. Definition of Hamiltonians in a Schrödinger representation

We take a Schrödinger representation instead of the Fock representation to apply functional integrals, i.e. we unitarily transform H_{PF} to H acting on the Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{F}$$

where $\mathcal{F} := L^2(Q, d\mu)$, and (Q, μ) denotes a probability space defined below. We assume that the quantum particle moves in the d -dimensional space to see dimensional dependences. Moreover, since taking the Coulomb gauge is irrelevant to the main subject and is not of major importance to our discussions, we do not stick to the Coulomb gauge and generalize polarization vectors.

We begin with some definitions often used in this paper. Let \mathbf{F} be the Fourier transform on $L^2(\mathbb{R}^\nu)$ for $\nu = d, d+1$, and $\hat{f} := \mathbf{F}f$ for $f \in L^2(\mathbb{R}^\nu)$. Moreover, for $f = f_1 \oplus \dots \oplus f_k \in \oplus^k L^2(\mathbb{R}^\nu)$ we set $\hat{f} := \hat{f}_1 \oplus \dots \oplus \hat{f}_k$. Define

$$W := \oplus^D L^2(\mathbb{R}^d) \quad W_0 := \oplus^D L^2(\mathbb{R}^d)$$

with a fixed D . Let \mathcal{E} be a bounded linear operator

$$\mathcal{E} : W \rightarrow W_0 \quad \|\mathcal{E}f\|_{W_0} \leq \beta \|f\|_W$$

with some $\beta > 0$. We suppose that \mathcal{E} is decomposable: $\mathcal{E} = \int_{\mathbb{R}^d}^{\oplus} \mathcal{E}(k) dk$ where $\mathcal{E}(k)$ is a linear operator $\mathcal{E} : \mathbb{C}^d \rightarrow \mathbb{C}^D$ such that $\mathcal{E}(k)k = 0$. This is a general version of Coulomb gauge conditions. Let

$$q(f, g) := (\mathcal{E}\hat{f}, \mathcal{E}\hat{g})_{W_0} \quad f, g \in W.$$

³ $(\cdot, \cdot)_{\mathcal{K}}$ denotes the scalar product on Hilbert space \mathcal{K} . We denote by $\|\cdot\|_{\mathcal{K}}$ the norm on \mathcal{K} . Unless confusion arises from the context we omit \mathcal{K} in $(\cdot, \cdot)_{\mathcal{K}}$ and $\|\cdot\|_{\mathcal{K}}$.

Let $L^2_{\text{real}}(\mathbb{R}^{\nu})$ be the set of real-valued L^2 -functions on \mathbb{R}^{ν} . Let $\phi(f)$ be the mean zero Gaussian random process [12] indexed by $f \in W_{\text{real}} := \oplus^d L^2_{\text{real}}(\mathbb{R}^d)$ on a probability measure space (Q, μ) with

$$\int_Q \phi(f)\phi(g) \, d\mu(\phi) = \frac{1}{2}q(f, g).$$

We extend $\phi(f)$ for $f \in W$ by

$$\phi(f) = \phi(\Re f) + i\phi(\Im f). \tag{2.1}$$

Let

$$\mathcal{F} := L^2(Q).$$

It is known that

$$\mathcal{F}_{\text{fin}} := \bigcup_{N=0}^{\infty} \oplus_{n=0}^N L\{\phi(f_1) \cdots \phi(f_n) \mid f_j \in W, j = 1, \dots, n\}$$

is dense in \mathcal{F} , where $:X:$ denotes the Wick product of X [24], $L\{\cdots\}$ the finite linear sum of vectors in $\{\cdots\}$, and $\oplus_{n=0}^0 L\{\cdots\} := \mathbb{C}$. We define the free Hamiltonian H_f in \mathcal{F} by

$$H_f \Omega := 0 \quad H_f : \phi(f_1) \cdots \phi(f_n) : = \sum_{j=1}^n : \phi(f_1) \cdots \phi(\langle \omega \rangle_d f_j) \cdots \phi(f_n) : \\ f_j \in D(\langle \omega \rangle_d) \quad j = 1, \dots, n \quad n \geq 1$$

where $D(T)$ denotes the domain of T and

$$\langle T \rangle_l := \oplus^l T.$$

The number operator is defined by

$$N_f \Omega := 0 \quad N_f : \phi(f_1) \cdots \phi(f_n) : := n : \phi(f_1) \cdots \phi(f_n) :.$$

It is well known that

$$\sigma(H_f) = [0, \infty), \quad \sigma_p(H_f) = \{0\}$$

and $\{0\}$ is simple with

$$H_f \Omega = 0.$$

The quantized radiation field $A(x) := (A_1(x), \dots, A_d(x))$ is defined by

$$A_{\mu}(x) := \sqrt{\hbar c} \phi(\lambda_{\mu}(\cdot - x)) \quad \mu = 1, \dots, d$$

where $\lambda_{\mu} := \oplus_{\nu=1}^d \delta_{\mu\nu} \lambda$. Then the Hamiltonian H_0 is given by

$$H_0 := \frac{1}{2} \left(p \otimes 1 - \frac{e}{c} A(x) \right)^2 + \hbar c 1 \otimes H_f.$$

For notational brevity we abbreviate $X \otimes 1$ and $1 \otimes X$ by X unless confusion arises.

Proposition 2.1. *Let λ be real and $\hat{\lambda}/\sqrt{\omega}, \omega\hat{\lambda} \in L^2(\mathbb{R}^d)$. Then for arbitrary $e \in \mathbb{R}$, H_0 is self-adjoint on $D(p^2) \cap D(H_f)$ and bounded from below.*

Proof. See [17]. □

Throughout this paper we assume

$$\lambda \text{ is real and } \hat{\lambda}/\sqrt{\omega}, \omega\hat{\lambda} \in L^2(\mathbb{R}^d).$$

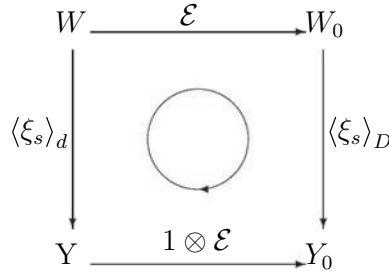


Figure 1. $\langle \xi_s \rangle_D \mathcal{E} = (1 \otimes \mathcal{E}) \langle \xi_s \rangle_d$.

Let $d = 3$, $D = d - 1 = 2$ and $\mathcal{E}(k) = \mathcal{E}_{\text{PF}}(k)$ be of the form

$$\mathcal{E}_{\text{PF}}(k) := \begin{pmatrix} e_1^1(k) & e_1^2(k) & e_1^3(k) \\ e_2^1(k) & e_2^2(k) & e_2^3(k) \end{pmatrix} : \mathbb{C}^3 \rightarrow \mathbb{C}^2 \quad k \in \mathbb{R}^3$$

where $\vec{e}_j(k) = (e_j^1(k), e_j^2(k), e_j^3(k))$. Moreover let λ be

$$\hat{\lambda}(k) = \frac{\hat{\rho}(k)}{\sqrt{(2\pi)^3 \omega(k)}}.$$

Then it is proved in [14] that there exists a unitary operator U from \mathcal{H} to \mathcal{H}_{PF} such that

$$U(H_0 + V)U^{-1} = H_{\text{PF}}.$$

2.2. Functional integral representations

For the reader's convenience and to state our results precisely, we give a functional integral representation of semigroup e^{-tH} , $t \geq 0$, following widely [14]. We denote by $\{\mathbf{b}(s)\}_{s \geq 0} = \{b_\mu(s)\}_{s \geq 0, 1 \leq \mu \leq d}$ the d -dimensional Brownian motion on the Wiener space $(C([0, \infty)), m)$. Set $M := \mathbb{R}^d \times C([0, \infty))$, $X_s := \mathbf{b}(s) + x$ and $dX := dx \otimes dm$. We define the family of isometries ξ_s , $s \in \mathbb{R}$ (figure 1)

$$\xi_s : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^{d+1})$$

by

$$\widehat{\xi_s f}(k, k_0) := \frac{e^{-isk_0}}{\sqrt{\pi}} \left(\frac{\omega(k)}{\omega(k)^2 + |k_0|^2} \right)^{1/2} \hat{f}(k) \quad (k, k_0) \in \mathbb{R}^d \times \mathbb{R}.$$

It is easily checked that

$$\xi_s^* \widehat{\xi_t f} = e^{-|t-s|\omega} \hat{f} \quad t, s \in \mathbb{R}.$$

Let

$$Y := \oplus^d L^2(\mathbb{R}^{d+1}) \cong L^2(\mathbb{R}) \otimes W \quad Y_0 := \oplus^D L^2(\mathbb{R}^{d+1}) \cong L^2(\mathbb{R}) \otimes W_0$$

and

$$q_0(f, g) := ((1 \otimes \mathcal{E})\hat{f}, (1 \otimes \mathcal{E})\hat{g})_{Y_0} \quad f, g \in Y.$$

Let $\phi_0(f)$ be the mean zero Gaussian random process indexed by $f \in \oplus^d L^2_{\text{real}}(\mathbb{R}^{d+1})$ on a probability measure space (Q_0, μ_0) with

$$\int \phi_0(f)\phi_0(g) d\mu_0(\phi_0) = \frac{1}{2}q_0(f, g)$$

$\phi_0(f)$ can be extended to $f \in Y$ in the same way as (2.1). Let

$$\mathcal{F}_0 := L^2(Q_0).$$

Then Ξ_s is defined by

$$\Xi_s \Omega := \Omega_0 \quad \Xi_s : \phi(f_1) \cdots \phi_n(f_n) := : \phi_0(\langle \xi_s \rangle_d f_1) \cdots \phi_0(\langle \xi_s \rangle_d f_n) :$$

where $\Omega_0 \equiv 1$ in \mathcal{F}_0 , so that $\Xi_s, s \in \mathbb{R}$, is the family of isometries

$$\Xi_s : \mathcal{F} \rightarrow \mathcal{F}_0$$

with

$$\Xi_s^* \Xi_t = e^{-|t-s|H_t} \quad t, s \in \mathbb{R}.$$

Definition 2.2. Let S be a closed subset of \mathbb{R}^d such that its Lebesgue measure is zero. We say that $V = V_+ - V_- \in \mathcal{P}(S)$ (where $V_+ := (V + |V|)/2$ and $V_- := (|V| - V)/2$) if V is such that

- (1) $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d \setminus S)$;
- (2) $D(p^2) \cap D(V_+)$ is dense in $L^2(\mathbb{R}^d)$;
- (3) V_- is infinitesimally small with respect to p^2 in $L^2(\mathbb{R}^d)$ in the sense of form.

In particular we set $\mathcal{P}(\emptyset) := \mathcal{P}_0$.

For $V \in \mathcal{P}(S)$, we define

$$H := H_0 \dot{+} V_+ \dot{-} V_- \tag{2.2}$$

where $\dot{\pm}$ denotes the quadratic form sum [20]. Let $V \in \mathcal{P}(S)$. Then, in [14, theorem 4.9], it is established that

$$(F, e^{-tH} G)_{\mathcal{H}} = \int_M dX e^{-(1/\hbar^2) \int_0^{\hbar^2 t} V(X_s) ds} (\Xi_0 F_0, e^{-i\phi_0(\mathcal{K})} \Xi_{\hbar c t} G_{\hbar^2 t})_{\mathcal{F}_0} \tag{2.3}$$

where

$$\mathcal{K} := \frac{e}{\sqrt{\hbar c}} \oplus_{\mu=1}^d \int_0^{\hbar^2 t} \xi_s \lambda(\cdot - X_s) db_{\mu}(s).$$

Here $\int_0^{\hbar^2 t} \dots db_{\mu}(s), \mu = 1, \dots, d$, are $L^2(\mathbb{R}^{d+1})$ -valued stochastic integrals, $F_t := F(X_t)$, and $G_s := G(X_s)$. In [14], (2.3) is proved only in the case of $S = \emptyset$. In the same manner as that of [27, theorem 6.2], it is also proved that (2.3) holds true in the case of $S \neq \emptyset$ but its Lebesgue measure is zero.

3. Embedded eigenvalues

In this section we put $\hbar = c = 1$. Let A and B be self-adjoint operators in a Hilbert space \mathcal{K} . We write $A \leq B$ if $D(B) \subset D(A)$ and $(f, Af) \leq (f, Bf)$ for all $f \in D(B)$.

3.1. Singular potentials

Let $D_j, j = 1, \dots, M$, be open sets in \mathbb{R}^d such that (1) $\overline{\cup_{j=1}^M D_j} = \mathbb{R}^d$, (2) $\cap_{j=1}^M D_j = \emptyset$, (3) the Lebesgue measure of $\partial(\cup_{j=1}^M D_j)$ is zero. Let

$$\mathcal{H}_j := L^2(D_j) \otimes \mathcal{F}.$$

We fix D_j 's throughout the present subsection.

Definition 3.1. We say that $V = V_+ - V_- \in \mathcal{P}_{\text{sing}}$ if for all $j = 1, \dots, M$,

- (1) $V \in \mathcal{P}(\partial(\cup_{j=1}^M D_j))$;
- (2) $\int_0^t V_+(X_s) ds = \infty$ for an arbitrary Wiener path such that $X_0 \in D_i$ and $X_t \in D_j$ with $i \neq j$;
- (3) $H_{p_j} := p^2/2 + V|_{L^2(D_j)}$ is essentially self-adjoint on $C_0^\infty(D_j)$, and there exist constants a and b such that, on $L^2(D_j)$,

$$p^2 \leq aH_{p_j} + b; \tag{3.1}$$
- (4) $E_j(0) := \inf \sigma(H_{p_j}) \in \sigma_{\text{disc}}(H_{p_j})$ (a normalized eigenvector for eigenvalue $E_j(0)$ is denoted by Ψ_j).

Lemma 3.2. Suppose that V satisfies (1) and (2) of definition 3.1. Let P_j be the projection of $L^2(\mathbb{R}^d)$ onto $L^2(D_j)$ and $\hat{p}_j := P_j \otimes 1$. Then $e^{-tH} \hat{p}_j = \hat{p}_j e^{-tH}$, $t \geq 0$.

Proof. Let $F := \psi \otimes \Psi \in C_0^\infty(\mathbb{R}^d) \hat{\otimes} \mathcal{F}$ and $G := \phi \otimes \Phi \in C_0^\infty(\mathbb{R}^d) \hat{\otimes} \mathcal{F}$, where $\hat{\otimes}$ denotes an algebraic tensor product. Let

$$M_t := \{X \in M \mid X_s \in D_i \text{ for all } 0 \leq s \leq t\}.$$

By definition 3.1 (2) and the fact that

$$\sup_{X \in M} |(\Xi_0 F_0, e^{-i\phi_0(K)} \Xi_t G_t)| < \infty$$

it holds that $(\Xi_0 F_0, e^{-i\phi_0(K)} \Xi_t G_t) = 0$ for each $X \in M$ such that $X_0 \in D_i$ and $X_t \in D_j$ with $i \neq j$, $e^{-\int_0^t V(X_s) ds}$. Hence

$$\begin{aligned} (F, e^{-tH} \hat{p}_j G) &= \sum_{i=1}^M \int_{Q_0} \overline{\Xi_0 \Psi} \Xi_t \Phi d\mu_0 \int_{M_i} e^{-\int_0^t V(X_s) ds} \overline{\psi(X_0)} (P_j \phi)(X_t) e^{-i\phi_0(K)} dX \\ &= \int_{Q_0} \overline{\Xi_0 \Psi} \Xi_t \Phi d\mu_0 \int_{M_j} e^{-\int_0^t V(X_s) ds} \overline{\psi(X_0)} (P_j \phi)(X_t) e^{-i\phi_0(K)} dX \\ &= \int_{Q_0} \overline{\Xi_0 \Psi} \Xi_t \Phi d\mu_0 \int_{M_j} e^{-\int_0^t V(X_s) ds} \overline{(P_j \psi)(X_0)} \phi(X_t) e^{-i\phi_0(K)} dX \\ &= (\hat{P}_j F, e^{-tH} G) = (F, \hat{P}_j e^{-tH} G). \end{aligned}$$

Thus the lemma follows. □

By lemma 3.2, we see that

$$H \hat{P}_j \subset \hat{P}_j H.$$

Thus

$$H_j := H|_{\mathcal{H}_j}$$

is self-adjoint in H_j with $D(H_j) = \mathcal{H}_j \cap D(H)$ and

$$H = \oplus_{j=1}^M H_j$$

under the identification

$$\mathcal{H} \cong \oplus_{j=1}^M \mathcal{H}_j.$$

Lemma 3.3. Let $V \in \mathcal{P}_{\text{sing}}$. Then there exists $e(V)$ such that, for $|e| \leq e(V)$, H_j is essentially self-adjoint on $\mathcal{D}_j := C_0^\infty(D_j) \hat{\otimes} \{\mathcal{F}_{\text{fin}} \cap D(H_f)\}$, $j = 1, \dots, M$, and bounded below. In particular H is essentially self-adjoint on $\oplus_{j=1}^M \mathcal{D}_j$.

Proof. Note that $H_{d_j} := H_{p_j} + H_f$ is essentially self-adjoint on \mathcal{D}_j by (3) of definition 3.1. Let $H_j = H_{d_j} + H_I$, where

$$H_I := \frac{1}{2}\{-2eA(x) \cdot p + e^2 A^2(x)\}.$$

From (3.1) and fundamental inequalities

$$\begin{aligned} \|A_\mu(x)\Psi\| &\leq C_1\left(\|\lambda/\sqrt{\omega}\| \|H_f^{1/2}\Psi\| + \|\lambda\|\|\Psi\|\right) \\ \|A_\mu^2(x)\Psi\| &\leq C_2(\|\lambda/\sqrt{\omega}\|^2 + \|\lambda\|^2)\|(H_f + I)\Psi\| \end{aligned}$$

with some constants C_1 and C_2 , it follows that, for $\Psi \in \mathcal{D}_j$

$$\|H_I\Psi\| \leq eA\|H_{d_j}\Psi\| + eB\|\Psi\|$$

with positive constants A and B . Let $e(V) := 1/A$. For $|e| < e(V)$ we obtain that \mathcal{D}_j is a core of H_j in \mathcal{H}_j by the Kato–Rellich theorem and hence $\bigoplus_{j=1}^M \mathcal{D}_j$ is a core of $H = \bigoplus_{j=1}^M H_j$. \square

Lemma 3.4. *Let $V \in \mathcal{P}_{\text{sing}}$. Then there exists $0 < e_g(V) < e(V)$ such that, for $|e| \leq e_g(V)$, a ground state, $\Psi_j(e)$, of H_j exists and is unique up to multiple constants. Moreover, if Ψ_j is the unique ground state of H_{p_j} , then $s - \lim_{e \rightarrow 0} \Psi_j(e) = \Psi_j(0) := \Psi_j \otimes \Omega$ in \mathcal{H}_j .*

Proof. We show an outline of a proof. In the same manner as in [6, 15] we show that $H_j + mN_f$, $m > 0$, has a ground state Ψ_j^m with $\|\Psi_j^m\|_{\mathcal{H}_j} = 1$ in \mathcal{H}_j . Let

$$Q_j := E_{H_{p_j}}([E_j(0), \epsilon]) \otimes E_{H_f}(\{0\})$$

where $E_T(\cdot)$ denotes the spectral projection of T and ϵ a positive constant such that $\dim \text{Ran } Q_j < \infty$. Taking a subsequence, $\{m_k\}_{k=1}^\infty$ ($m_k \downarrow 0$ as $k \rightarrow \infty$), we see that $\Psi_j^{m_k}$ weakly converges to vector $\hat{\Psi}_j$ and that

$$(\hat{\Psi}_j, Q_j \hat{\Psi}_j) \geq 1 - \Delta_j(e) \tag{3.2}$$

where $\Delta_j(e)$ denotes a positive function such that $\Delta_j(e) \rightarrow 0$ as $e \rightarrow 0$. It follows from (3.2) that $\hat{\Psi}_j \neq 0$ for sufficiently small $|e|$. Hence $\Psi_j(e) := \hat{\Psi}_j$ is a ground state of H_j for such small e 's. It is proved in [15] that

$$e^{-i\pi N_f/2} e^{-tH_j} e^{i\pi N_f/2}$$

is positivity improving in \mathcal{H}_j . Hence the ground state of H_j is unique in \mathcal{H}_j . Since by (3.2), taking ϵ such that $\dim \text{Ran } Q_j = 1$, we see that $\|\Psi_j(e) - \Psi_j(0)\|^2 \leq 2\Delta_j(e)$, the last assertion follows. \square

The following lemma is well known:

Lemma 3.5. *Let $V \in \mathcal{P}_{\text{sing}}$ and $|e| \leq e(V)$. Then $\sigma_{\text{ess}}(H) = [\inf \sigma(H), \infty)$.*

Proof. See [3, theorem 1.3]. \square

Let $E \in \sigma_p(T)$. Then we denote by $m_T(E)$ the multiplicity of E .

Theorem 3.6. *Let $V \in \mathcal{P}_{\text{sing}}$ and $|e| \leq e_g(V)$. Set*

$$E_j := \inf \sigma(H_j) \quad j = 1, \dots, M.$$

Then $E_j \in \sigma_p(H) \subset \sigma_{\text{ess}}(H)$ and

$$m_H(E_j) \geq \#\{E_k | E_k = E_j, k = 1, \dots, M\}. \tag{3.3}$$

Moreover $\lim_{e \rightarrow 0} E_j = E_j(0)$.

Proof. Since $H \simeq \bigoplus_{j=1}^M H_j$, we see that $\bigoplus_{i=1}^M \delta_{ij} \Psi_j(e)$ is an eigenvector of H with eigenvalue E_j . Then (3.3) follows. It is easily seen that $H_j \rightarrow H_{dj}$ in the uniform resolvent sense in \mathcal{H}_j as $e \rightarrow 0$. Then $\lim_{e \rightarrow 0} E_j = E_j(0)$. Thus the theorem follows. \square

Corollary 3.7. *Let $V \in \mathcal{P}_{\text{sing}}$ and $|e| \leq e_g(V)$. Define*

$$E := \min_k E_k = \inf \sigma(H).$$

Let

$$H(j_1, \dots, j_k) := H - E - \sum_{l=1}^k (E_{j_l} - E) \chi_{D_{j_l}}$$

where $j_l \in \{1, \dots, N\}$, $j_n \neq j_m, n \neq m$, and χ_B is the characteristic function of $B \subset \mathbb{R}^d$. Then $H(j_1, \dots, j_k)$ has ground states with eigenvalue zero and

$$m_{H(j_1, \dots, j_k)}(0) \geq k.$$

In particular

$$H(1, \dots, M) = H - \sum_{j=1}^M E_j \chi_{D_j}$$

has ground states and

$$m_{H(1, \dots, M)}(0) = M.$$

Proof. By lemma 3.2, we see that $H(j_1, \dots, j_k) = \bigoplus_{j=1}^M H_j(j_1, \dots, j_k)$, where

$$H_j(j_1, \dots, j_k) := \begin{cases} H_j - E & j \notin \{j_1, \dots, j_k\} \\ H_j - E_j & j \in \{j_1, \dots, j_k\}. \end{cases}$$

Hence $\hat{\Psi}_{j_l}, l = 1, \dots, k$, are ground states. Thus $m_{H(j_1, \dots, j_k)}(0) \geq k$ follows. Since each ground state of H_j is unique in \mathcal{H}_j , it follows that $m_{H(1, \dots, M)}(0) = M$. \square

3.2. Examples

In this subsection we give an example of H having embedded eigenvalues and degenerate eigenvectors. Let $d = 3$ and $\hat{\lambda}(-k) = \hat{\lambda}(k)$. We define

$$\begin{aligned} \Omega_1 &:= \{x \in \mathbb{R}^3 | x_1 > 0, x_2 > 0, x_3 > 0\} \\ \Omega_2 &:= \{x \in \mathbb{R}^3 | x_1 < 0, x_2 < 0, x_3 < 0\} \\ \Omega_3 &:= \mathbb{R}^3 \setminus \overline{\Omega_1 \cup \Omega_2}. \end{aligned}$$

Set $\Omega := \bigcup_{i=1}^3 \Omega_i$. Let

$$V_v(x) := \frac{v}{|x - \partial\Omega|^3} + |x|^2 + m \chi_{\Omega_1} + n \chi_{\Omega_2}$$

where v, m , and n are constants (see figures 2 and 3). Let

$$H_p(v) := p^2/2 + V_v \quad D(H_p(v)) := C_0^\infty(\Omega) \quad H(v) := \frac{1}{2}(p - eA(x))^2 + H_f + V_v.$$

Lemma 3.8. *Let $H_{p_j}(v) := H_p(v)|_{D_j}$. Then, for all $v > 0$, $H_{p_j}(v), j = 1, 2, 3$, are essentially self-adjoint on $C_0^\infty(\Omega_j)$.*

Before proving lemma 3.8 we show a general lemma as follows:

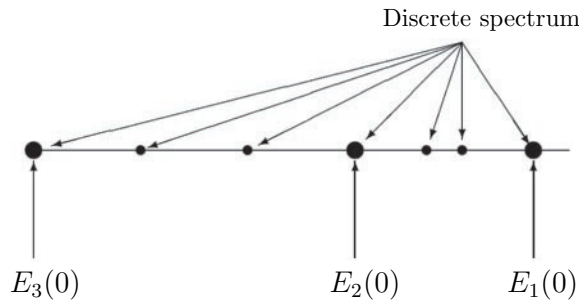


Figure 2. The spectrum of $H_p(v)$ for $1 \ll n < m$.

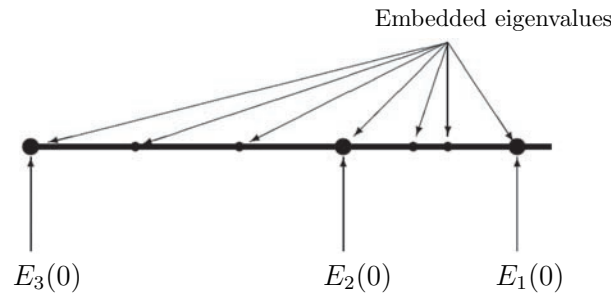


Figure 3. The spectrum of $H_d(v) := H_p(v) + H_f$ for $1 \ll n < m$.

Lemma 3.9. Let G be an open set in \mathbb{R}^d and $V \geq 0$ on G . We assume that there exists a uniform Lipschitz function σ on every compact subset in G such that

- (1) $\sum_{i=1}^d (\partial_i \sigma)^2 \leq e^{2\sigma}$ almost everywhere on G ;
- (2) $\lim_{x \rightarrow \partial G} \sigma(x) = \infty$, where if G is not bounded, ∞ is regarded as a point of ∂G ;
- (3) there exists $\delta > 0$ such that $(u, (p^2 + V)u) \geq (1 + \delta)(u, e^{2\sigma}u)$ for $u \in C_0^\infty(G)$.

Then $p^2 + V$ is essentially self-adjoint on $C_0^\infty(G)$.

Proof. See [21, 30].

Proof of Lemma 3.8. Fix j . It is enough to prove essential self-adjointness of $H_{p_j}(v)$ for $n = m = 0$. Let

$$V_j(x) := \frac{v}{|x - \partial\Omega_j|^3} + |x|^2$$

and

$$V(x) := V_\epsilon(x) + |x|^2$$

where

$$V_\epsilon(x) := \begin{cases} v/|x - \partial\Omega_j|^3 & |x - \partial\Omega_j| < \epsilon \\ v/\epsilon^3 & \text{otherwise} \end{cases}$$

where ϵ will be adjusted below. We shall prove essential self-adjointness of $p^2 + 2V$ on $C_0^\infty(\Omega_j)$. It implies that $p^2 + 2V_j$ is essentially self-adjoint on $C_0^\infty(\Omega_j)$, since $V_j = V_\epsilon +$ (a bounded operator). It is sufficient to find a function corresponding to σ in lemma 3.9. Let

$$\sigma_\epsilon := \log V_\epsilon^{1/2}.$$

It is easily seen that σ_j is a uniform Lipschitz function on every compact subset in Ω_j . Since $(u, (p^2 + 2V)u) \geq (u, 2Vu) = 2(u, e^{2\sigma_\epsilon} u)$ for all $u \in C_0^\infty(\Omega_j)$ and $\lim_{x \rightarrow \partial\Omega_j} \sigma_\epsilon(x) = \infty$, (2) and (3) in lemma 3.9 are checked. (1) in lemma 3.9 is equivalent to $0 \leq 4V_\epsilon^3 - \sum_{i=1}^d (\partial_i V_\epsilon)^2$. By a direct calculation we see that, for $x \in \mathbb{R}^d$ such that $|x - \partial\Omega_j| < \epsilon$,

$$4V_\epsilon^3 - \sum_{i=1}^d (\partial_i V_\epsilon)^2 \geq 4 \left(\frac{v}{|x - \partial\Omega_j|^3} + |x|^2 \right)^3 - \frac{1}{2} \left(\frac{9v^2}{|x - \partial\Omega_j|^8} + 4|x|^2 \right) > 2(\mathcal{V}_1 + \mathcal{V}_2)$$

where

$$\mathcal{V}_1(x) := \frac{2v^3}{|x - \partial\Omega_j|^8} \left(\frac{1}{|x - \partial\Omega_j|} - \frac{9}{4v} \right) \quad \mathcal{V}_2(x) := |x|^2(2|x|^4 - 1).$$

Thus taking ϵ sufficiently small, we have $\mathcal{V}_1 + \mathcal{V}_2 > 0$. Moreover, for $x \in \mathbb{R}^d$ such that $|x - \partial\Omega_j| > \epsilon$, it is clear that

$$4V_\epsilon^3 - \sum_{i=1}^d (\partial_i V_\epsilon)^2 = 4V_\epsilon^3 \geq 0.$$

Thus $p^2 + 2V$ is essentially self-adjoint on $C_0^\infty(\Omega_j)$ and then $H_{p_j}(v)$ is also essentially self-adjoint on $C_0^\infty(\Omega_j)$. \square

Lemma 3.10. *Let $v > 0$. Then $V_v \in \mathcal{P}_{\text{sing}}$. Moreover, the ground state of $H_{p_j}(v)$, $j = 1, 2, 3$, is unique in $L^2(D_j)$.*

Proof. In this proof essential ingredients are from [9, 15]. It is enough to prove the lemma for $n = m = 0$. It is clear that $V_v \in L_{\text{loc}}^1(\mathbb{R}^d \setminus \partial\Omega)$. By lemma 3.8, H_{p_j} is essentially self-adjoint on $C_0^\infty(\Omega_j)$, and for arbitrary Wiener path such that $X_0 \in \Omega_i$ and $X_t \in \Omega_j$, $i \neq j$, $\int_0^t V_v(X_s) ds = \infty$. Since V_v is positive, we have $(f, p^2 f)_{L^2(D_j)} \leq (f, H_{p_j} f)_{L^2(D_j)}$ for $f \in C_0^\infty(\Omega_j)$. Note that $p^2/2 + |x|^2$ has a purely discrete spectrum and that $p^2/2 + |x|^2 \leq H_{p_j}(v)$. Since $H_p(v) = \oplus_{j=1}^3 H_{p_j}(v)$, from the min-max principle [26], it follows that $H_{p_j}(v)$ has a purely discrete spectrum. Then $V_v \in \mathcal{P}_{\text{sing}}$. Finally since

$$e^{i\pi N_t/2} e^{-tH_{p_j}(v)} e^{-i\pi N_t/2}$$

is positivity improving on $L^2(\Omega_j)$, the ground state of $H_{p_j}(v)$ is unique in $L^2(\Omega_j)$. Thus the lemma follows. \square

By lemma 3.2 we have $H(v) = \oplus_{i=1}^3 H_i(v)$, where $H_i(v) = H(v)|_{L^2(\Omega_i) \otimes \mathcal{F}}$.

Lemma 3.11. *Let $v > 0$. Let $|e|$ be sufficiently small. Set $E_j := \inf \sigma(H_j(v))$, $j = 1, 2, 3$. Then (1) $E_1 = E_2$ if $n = m$; (2) $E_3 < E_2 < E_1$ if $n < m$ and n is sufficiently large; (3) $E_1 < E_2 < E_3$ if $m < n$ and n is sufficiently small (see figure 4 and 5).*

Proof. Let $E_j(0) := \inf \sigma(H_{p_j}(v))$, $j = 1, 2, 3$. Taking sufficiently large n , we see that $E_3(0) < E_2(0) < E_1(0)$. Then, from theorem 3.6, it follows that $E_3 < E_2 < E_1$ for sufficiently small $|e|$. Thus (2) follows. Equation (3) is similarly proved. Let $n = m$. Define $S : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ by

$$Sf(x) := f(-x)$$

and $T := \mathbf{F}S\mathbf{F}^{-1}$, where \mathbf{F} is the Fourier transform. We define unitary operator

$$\mathbf{U} := S|_{L^2(\Omega_2)} \otimes \mathbf{T} : L^2(\Omega_2) \otimes \mathcal{F} \rightarrow L^2(\Omega_1) \otimes \mathcal{F}$$

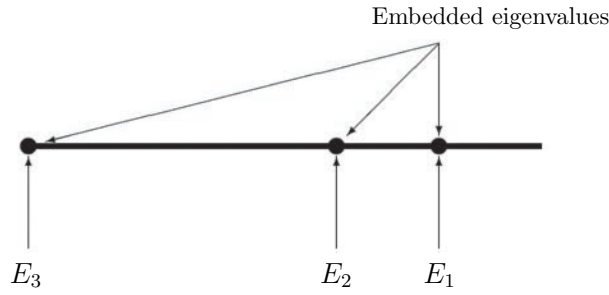


Figure 4. The spectrum of $H(v)$ for $1 \ll n < m$.

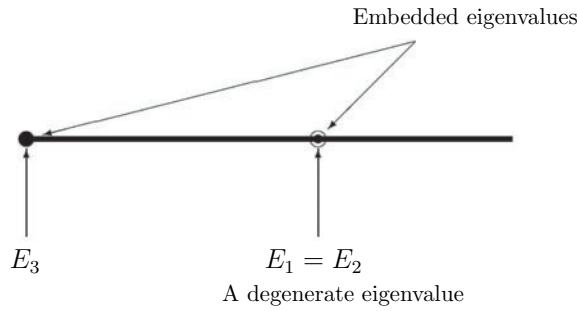


Figure 5. The spectrum of $H(v)$ for $1 \ll n = m$.

where $\mathbf{T}:\phi(f_1) \cdots \phi(f_n) := \phi(Tf_1) \cdots \phi(Tf_n)$ and $\mathbf{T}\Omega := \Omega$. Since $\lambda(-k) = \lambda(k)$

$$\mathbf{U}^{-1}A_\mu(x)\mathbf{U} = A_\mu(x).$$

Moreover we see that

$$\mathbf{U}^{-1}p_\mu\mathbf{U} = -p_\mu \quad \mathbf{U}^{-1}V_1\lceil_{L^2(\Omega_1)}\mathbf{U} = V_2\lceil_{L^2(\Omega_2)}$$

and

$$\mathbf{U}^{-1}H_f\mathbf{U} = H_f.$$

Hence

$$\mathbf{U}^{-1}H_1(v)\mathbf{U} = \frac{1}{2}(p + eA(x))^2 + V_2 + H_f := \tilde{H}_2(v).$$

Since $(f \otimes \Omega, \Psi_g) \neq 0$,

$$\begin{aligned} \inf \sigma(H_2(v)) &= - \lim_{t \rightarrow \infty} \frac{1}{t} \log(f \otimes \Omega, e^{-tH_2(v)} f \otimes \Omega) \\ &= - \lim_{t \rightarrow \infty} \frac{1}{t} \log \int_M f(X_0)f(X_t)e^{-e^2q_0(K)/4} dX. \end{aligned}$$

Hence $\inf \sigma(H_2(v))$ is invariant on $e \rightarrow -e$, $\inf \sigma(\hat{H}_2(v)) = \inf \sigma(H_2(v))$. Hence $E_2 = E_1$. □

Theorem 3.12. *Let $v > 0$. Let $|e|$ be sufficiently small and $E := \min_{j=1,2,3} E_j$. Then $\sigma_{\text{ess}}(H(v)) = \sigma(H(v)) = [E, \infty)$ and $E_j \in \sigma_p(H(v))$, $j = 1, 2, 3$. Moreover (1) $m_{H(v)}(E_j) = 1$, $j = 1, 2, 3$, if $n \neq m$, and $|n|$ and $|m|$ are sufficiently large; (2) $m_{H(v)}(E_1 = E_2) = 2$, if $n = m$ and $|n|$ is sufficiently large; (3) $\lim_{e \rightarrow 0} E_j = E_j(0)$, $j = 1, 2, 3$ (see figure 6).*

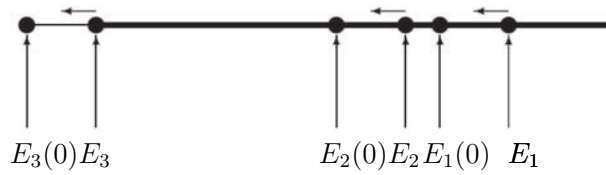


Figure 6. $\lim_{\epsilon \rightarrow 0} E_j = E_j(0)$.

Proof. It follows from lemmas 3.5, 3.10, and 3.11. □

We give two remarks.

- (1) In case (2) in theorem 3.12 for $n = m$ with n sufficiently small, $H(v)$ has twofold ground states.
- (2) By a functional integral representation, we have

$$s - \lim_{v \rightarrow 0} (F, e^{-tH(v)} G) = \sum_{j=1}^3 \int_{M_j} dX e^{-\int_0^t |X_s|^2 ds} (\Xi_0 \Psi(X_0), \Xi_t \Phi(X_t)) \neq (F, e^{-tH(0)} G).$$

Hence we observe a Klauder phenomenon [8, 22]:

$$s - \lim_{v \rightarrow 0} e^{-tH(v)} \neq e^{-tH(0)}.$$

This phenomenon carries an interesting consequence that once turned on an effect of a singular potential cannot be completely turned off.

4. Localization of charge densities

4.1. Localization I

In the present section we shall show an exponential decay of a charge density of eigenvectors Ψ_p of H . We set

$$\mathbf{J}_t := \Xi_0^* e^{-ie\phi_0(K)} \Xi_t.$$

Assume that

$$H\Psi_p = E\Psi_p.$$

Let Δ be the cube with the unit side centred about the origin in \mathbb{R}^d . We say that $f \in L^p_u(\mathbb{R}^d)$ if

$$\|f\|_{L^p_u(\mathbb{R}^d)}^p := \sup_{x \in \mathbb{R}^d} \int_{\Delta} |f(x+y)|^p dy < \infty.$$

Let us define $\mathbf{V}_{\text{bound}}$ and \mathbf{V}_{exp} by

$\mathbf{V}_{\text{bound}}$: $V = V_+ - V_-$, such that $V_{\pm} \geq 0$, $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$ and $V_- = \sum_{j=1}^J W_j$ such that $\sup_{z_j \in \mathbb{R}^{d-\mu_j}} \|W_j(\cdot, z_j)\|_{L^p_u(\mathbb{R}^{\mu_j})} < \infty$ for some $\mu_j, j = 1, \dots, J$.

\mathbf{V}_{exp} : $V = Z + W$, such that $Z \in L^1_{\text{loc}}(\mathbb{R}^d)$, and $W < 0$, $W \in L^p(\mathbb{R}^d)$ for some $p > \max\{1, d/2\}$.

Definition 4.1. Suppose $V = Z + W \in \mathbf{V}_{\text{exp}}$ and $V \in \mathbf{V}_{\text{bound}}$.

- (1) We say $V \in V(m)$, $m \geq 1$, if $Z(x) \geq \gamma|x|^{2m}$ outside a compact set for some positive constant γ .
- (2) We say $V \in V(0)$ if $\liminf_{|x| \rightarrow \infty} W(x) > \inf \sigma(H)$.

Lemma 4.2. *Let $V \in \mathbf{V}_{\text{bound}}$. Then $\sup_{x \in \mathbb{R}^d} \|\Psi_p(x)\| < \infty$.*

Proof. Let \mathbb{E} refer to the expectation value with respect to b . We have

$$\Psi_p = e^{tE} e^{-tH} \Psi_p = e^{tE} \mathbb{E} \left(\mathbf{J}_t e^{-\int_0^t V(X_s) ds} \Psi_p(X_t) \right).$$

Hence

$$\|\Psi_p(x)\| \leq e^{tE} \mathbb{E} \left(e^{-\int_0^t V(X_s) ds} \|\Psi_p(X_t)\| \right) = e^{tE} (e^{-tH_p} \|\Psi_p(\cdot)\|)(x).$$

Since by the assumption on V , $(e^{-tH_p} \|\Psi_p(\cdot)\|) \in L^\infty(\mathbb{R}^d)$ ([27, theorem 25.5, corollary 25.6]), we get the desired result. \square

Lemma 4.3. *Let $V \in \mathbf{V}_{\text{bound}} \cap \mathbf{V}_{\text{exp}}$. Then, for all $f \in C_0^\infty(\mathbb{R}^d)$ and $t > 0$,*

$$\int_{\mathbb{R}^d} f(x) \|\Psi_p(x)\|^2 dx \leq C e^{tE} \int_{\mathbb{R}^d} dx |f(x)| \mathbb{E} \left(e^{-\int_0^t V(X_s) ds} \right),$$

where $C := \sup_{x \in \mathbb{R}^d} \|\Psi_p(x)\|^2 < \infty$.

Proof. We see that, by lemma 4.2,

$$\begin{aligned} \int_{\mathbb{R}^d} f(x) \|\Psi_p(x)\|^2 dx &= (\bar{f} \Psi_p, \Psi_p)_{\mathcal{H}} = e^{tE} (\bar{f} \Psi_p, e^{-tH} \Psi_p) \\ &= e^{tE} \int_M dX f(x) e^{-\int_0^t V(X_s) ds} (\Psi_p(X_0), \mathbf{J}_t \Psi_p(X_t)) \\ &\leq e^{tE} \int_{\mathbb{R}^d} dx |f(x)| \mathbb{E} \left(\|\Psi_p(x)\| \|\Psi_p(X_t)\| e^{-\int_0^t V(X_s) ds} \right) \\ &\leq e^{tE} \sup_{x \in \mathbb{R}^d} \|\Psi_p(x)\|^2 \int_{\mathbb{R}^d} dx |f(x)| \mathbb{E} \left(e^{-\int_0^t V(X_s) ds} \right). \end{aligned}$$

Thus the lemma follows. \square

Theorem 4.4.

(1) *Suppose $V \in V(m)$, $m \geq 1$. Then for each sufficiently small positive constant δ , there exists a positive constant $D(\delta)$ such that*

$$\|\Psi_p(x)\| \leq D(\delta) \exp(-\delta|x|^{m+1}). \tag{4.1}$$

(2) *Suppose $V \in V(0)$. Then there exists a positive constant D and δ such that*

$$\|\Psi_p(x)\| \leq D e^{-\delta|x|}.$$

Proof. By [7, lemma 3.1] we see that, for sufficiently small δ , there exists $D(\delta)'$ such that

$$\mathbb{E} \left(e^{-\int_0^t V(X_s) ds} \right) \leq D(\delta)' e^{-\delta|x|^{m+1}}$$

for $|x| > N$ with some sufficiently large N . Let $D(\delta)'' := \sup_{|x| > N} C e^{tE} D(\delta)'$, where C is defined in lemma 4.3. By lemma 4.3 we see that, for all $f \in C_0^\infty(\mathbb{R}^d)$ with $f \geq 0$,

$$\int_{\{|x| > N\}} f(x) \left(\|\Psi_p(x)\|^2 - D(\delta)'' e^{-\delta|x|^{m+1}} \right) dx < 0.$$

Thus (4.1) holds for $|x| > N$. By lemma 4.2 $\|\Psi_p(x)\|$ is bounded. Thus (1) follows. We prove (2) in a similar way as (1) and [7, proposition 4.1]. Hence we omit it. \square

4.2. Localization II

From (2.3), an extension of Kato’s comparing inequality follows:

Proposition 4.5. *Let $V \in \mathcal{P}_0$. We assume that $\psi \in Q(p^2 \dot{+} V)$, $\psi \geq 0$, and $G \in D(H)$. Then $\|G(\cdot)\|_{\mathcal{F}} \in Q(p^2 \dot{+} V)$ and*

$$\Re((\text{sgn}G)(\psi \otimes 1), HG)_{\mathcal{H}} \geq \frac{1}{2}((p^2 \dot{+} V)^{1/2}\psi, (p^2 \dot{+} V)^{1/2}\|G(\cdot)\|_{\mathcal{F}})_{L^2(\mathbb{R}^d)}$$

where

$$\text{sgn}G(x) := \begin{cases} G(x)/\|G(x)\|_{\mathcal{F}} & \|G(x)\|_{\mathcal{F}} \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

is a multiplication operator and $Q(T)$ denotes the form domain of T . □

Proof. See [14].

Theorem 4.6. *Let $d = 3$. Suppose that hypothesis **S**, $D(H) \subset D(p^2)$, and*

$$E < \liminf_{|x| \rightarrow \infty} V(x) := V_0 \leq \infty.$$

Then there exist constants A and A_N such that

$$\|\Psi_p(x)\| \leq Ae^{-\sqrt{V_0-E}|x|} \quad V_0 < \infty$$

$$\|\Psi_p(x)\| \leq A_Ne^{-\sqrt{N-E}|x|} \quad V_0 = \infty$$

where N is an arbitrary number such that $N > E$.

Proof. We prove for the case of $V_0 < \infty$. For the case of $V_0 = \infty$, it is similarly proved. By assumption there exists R such that

$$V(x) - E > 0 \quad x \in B_R := \{y \in \mathbb{R}^3 \mid |y| > R\}.$$

Let $\psi \in C_0^\infty(B_R)$ with $\psi \geq 0$. By proposition 4.5 we have

$$\left(-\frac{1}{2}p^2\psi, \|\Psi_p(\cdot)\|\right) \geq (\psi, (V_0 - E)\|\Psi_p(\cdot)\|) \geq 0. \tag{4.2}$$

Let $\phi(x) := qe^{-\sqrt{V_0-E}|x|}$, where constant q will be adjusted below. A direct calculation shows that

$$-\frac{1}{2}p^2\phi(x) \leq (V_0 - E)\phi(x). \tag{4.3}$$

Since $d = 3$ and $G \in D(p^2)$, $G(x)$ is continuous in x and $\|\Psi_p(x)\| \rightarrow 0$ as $|x| \rightarrow \infty$ by the Sobolev lemma. In particular, $\|\Psi_p(x)\|$ is continuous in x . Thus taking sufficiently large q , we see that $u(x) := \|\Psi_p(x)\| - \phi(x) \leq 0$ for $x \in \partial B_R$. Fix such q . We see that, by (4.2) and (4.3)

$$\left(-\frac{1}{2}p^2\psi, u\right) \geq 0$$

for $\psi \in C_0^\infty(B_R)$ with $\psi \geq 0$. Hence u is subharmonic on B_R in the sense of distribution: $-p^2u \geq 0$ on B_R . Therefore $u|_{B_R}$ takes its maximum value on $\partial B_R \cup \{\infty\}$. Since $u(x) \rightarrow 0$ as $|x| \rightarrow \infty$ and $u|_{\partial B_R} < 0$, it holds that $u(x) \leq 0$ for $x \in B_R$. Hence $\|G(x)\| \leq qe^{-\sqrt{V_0-E}|x|}$ for $x \in B_R$. Thus the theorem follows from the continuity of $\|G(\cdot)\|$. □

5. Asymptotics

In this section we consider asymptotic behaviour of e^{-tH} . Especially we investigate classical and nonrelativistic limits. Throughout this section we assume

$$V \in \mathcal{P}_0.$$

5.1. Nonrelativistic limits

In this subsection we consider the nonrelativistic limit of e^{-tH} . Let P_Ω be the projection of \mathcal{F} onto $\{\mathbb{C}\Omega\}$.

Lemma 5.1. *Let $\Psi = F \otimes e^{i\phi(f)}$ and $\Phi = G \otimes e^{i\phi(g)}$, where $F, G \in C_0^\infty(\mathbb{R}^d)$ and $f, g \in W_{\text{real}}$. Then $\lim_{c \rightarrow \infty} (\Psi, e^{-tH} \Phi) = (\Psi, (e^{-tH_p} \otimes P_\Omega) \Phi)$.*

Proof. We have

$$(\Psi, e^{-tH} \Phi) = \int_M dX e^{-(1/\hbar^2) \int_0^{h^2 t} V(X_s) ds} \overline{F(X_0)} G(X_{hct}) e^{-\Theta/4}$$

where $\Theta := q_0(\mathcal{K} - \xi_0 f + \xi_{hct} g) := \text{I} + \text{II} + \text{III}$, and $\text{I} := q_0(\mathcal{K})$, $\text{II} := q_0(\xi_0 f - \xi_{hct} g)$, $\text{III} := 2\Re q_0(\mathcal{K}, \xi_{hct} g - \xi_0 f)$. It is well known that

$$\mathbb{E} (q_0(\mathcal{K})^{2m}) < \left(\frac{e}{\sqrt{\hbar c}} \right)^{2m} \frac{(2m)!}{2^m} t^{m-1} (d\beta)^{2m} \|\lambda\|_{L^2(\mathbb{R}^d)}^{2m}$$

by [17, lemma 4.4]. We see that $\lim_{c \rightarrow \infty} \mathbb{E}(\text{I}^2) = 0$, hence $\lim_{c \rightarrow \infty} \mathbb{E}(\text{III}^2) = 0$, while we have $\lim_{c \rightarrow \infty} \mathbb{E}(\text{II}^2) = (q(g) + q(f))^2$. Thus $\mathbb{E}\Theta^2 \rightarrow (q(g) + q(f))^2$ as $c \rightarrow \infty$. Similarly we have $\mathbb{E}\Theta \rightarrow q(g) + q(f)$ as $c \rightarrow \infty$. Hence

$$\lim_{c \rightarrow \infty} \mathbb{E} |e^{-\Theta/4} - e^{-q(f)/4} e^{-q(g)/4}|^2 \leq \lim_{c \rightarrow \infty} \mathbb{E} |\Theta - (q(g) + q(f))|^2 / 16 = 0.$$

Thus

$$\begin{aligned} \mathbb{E} \left| e^{-(1/\hbar^2) \int_0^{h^2 t} V(X_s) ds} \overline{F(X_0)} G(X_{hct}) (e^{-\Theta/4} - e^{-q(f)/4} e^{-q(g)/4}) \right| &\leq \|F\|_\infty \|G\|_\infty \\ &\times \left(\mathbb{E} e^{-(2/\hbar^2) \int_0^{h^2 t} V(X_s) ds} \right)^{1/2} \left(\mathbb{E} |e^{-\Theta/4} - e^{-q(f)/4} e^{-q(g)/4}|^2 \right)^{1/2} \rightarrow 0 \end{aligned}$$

as $c \rightarrow \infty$. Thus the lemma follows. □

Theorem 5.2. *We have $s - \lim_{c \rightarrow \infty} e^{-tH} = e^{-tH_p} \otimes P_\Omega$.*

Proof. It is sufficient to show that $s - \lim_{c \rightarrow \infty} (F, e^{-tH} G) = (F, e^{-tH_p} \otimes P_\Omega G)$ for F, G in a dense subset. Let

$$\mathcal{D} := \left\{ F := \int_{\mathbb{R}^n} \hat{F}(\vec{t}) e^{i \sum_{j=1}^n t_j \phi(f_j)} d\vec{t} \in \mathcal{F} \mid F \in \mathcal{S}(\mathbb{R}^n), f_j \in W_{\text{real}}, j = 1, \dots, n, n \in \mathbb{N} \right\}$$

where $\mathcal{S}(\mathbb{R}^n)$ denotes the set of Schwartz test functions on \mathbb{R}^n . Then $C_0^\infty(\mathbb{R}^d) \hat{\otimes} \mathcal{D}$ is dense in \mathcal{H} . Thus the theorem follows from lemma 5.1. □

5.2. Classical limits

In this subsection we discuss a classical limit of a partial trace of e^{-tH} . Let $\alpha(t) = \{\alpha_\mu(t)\}_{1 \leq \mu \leq d, 0 \leq t \leq 1}$ be the d -dimensional Brownian bridge on a probability measure space (B, α) , i.e., the mean zero Gaussian random process with the covariance

$$E_\alpha(\alpha_\mu(s) \alpha_\nu(t)) = \delta_{\mu\nu} s(1-t) \quad 0 \leq s \leq t \leq 1$$

where E_α refers to the expectation value with respect to (B, α) . Let

$$\mathcal{G} := \{g \in C_b^1(\mathbb{R}^d; L^2(\mathbb{R}^d)) \mid g(x) \in D(\omega), (\omega g)(\cdot) \in C_b^0(\mathbb{R}^d; L^2(\mathbb{R}^d))\}$$

where $C_b^n(\mathbb{R}^d; \mathcal{K})$ denotes the set of \mathcal{K} -valued n -times differentiable continuous functions to be bounded up to n -times derivative. Let $\Delta_k := (k - 1)t/2^n$. We set

$$B_n^\mu(g) := \sum_{k=1}^{2^n} \xi_{\Delta_k} g(\alpha(\Delta_k)) \{ \alpha_\mu(\Delta_{k+1}) - \alpha_\mu(\Delta_k) \}$$

$$= S_n^\mu(g) + \sum_{k=1}^{2^n} \xi_{\Delta_k} g(\alpha(\Delta_k)) \alpha_\mu(\Delta_k) (t/2^n)(1 - \Delta_k)^{-1}$$

where

$$S_n^\mu(g) := \sum_{k=1}^{2^n} \xi_{\Delta_k} g(\alpha(\Delta_k)) \gamma_\mu(t/2^n, \Delta_k)$$

with

$$\gamma_\mu(t, \Delta t) := \alpha_\mu(t + \Delta t) - \alpha_\mu(t) + \Delta t(1 - t)^{-1} \alpha_\mu(t).$$

Lemma 5.3. *Let $g \in \mathcal{G}$. Then the strong limit of $B_n^\mu(g)$ exists as $n \rightarrow \infty$ in $L^2(B; L^2(\mathbb{R}^{d+1}))$.*

Proof. In the similar manner as that of [14, theorem 2.5], it is shown that $S_n^\mu(g)$ strongly converges in $L^2(B; L^2(\mathbb{R}^{d+1}))$ as $n \rightarrow \infty$. While, since, for each path α , $\xi_s g(\alpha(s))$ is strongly continuous in $s \in \mathbb{R}$ in $L^2(\mathbb{R}^{d+1})$, we have, for each path α ,

$$s - \lim_{n \rightarrow \infty} \sum_{k=1}^{2^n} \frac{t}{2^n} \xi_{\Delta_k} g(\alpha(\Delta_k)) \alpha_\mu(\Delta_k) (1 - \Delta_k)^{-1} = \int_0^t \alpha_\mu(s) \xi_s g(\alpha(s)) (1 - s)^{-1} ds$$

in $L^2(\mathbb{R}^{d+1})$. Thus the proof is complete. □

We set $S_\infty^\mu(g) := s - \lim_{n \rightarrow \infty} S_n^\mu(g)$ in $L^2(B; L^2(\mathbb{R}^{d+1}))$. We define

$$\int_0^t \xi_s g(\alpha(s)) d\alpha_\mu(s) := S_\infty^\mu(g) + \int_0^t \alpha_\mu(s) \xi_s g(\alpha(s)) (1 - s)^{-1} ds \quad \mu = 1, \dots, d.$$

Lemma 5.4. *We have*

$$(F, e^{-tH} G)_{\mathcal{H}} = \int_{\mathbb{R}^{2d} \times B} dx dy d\alpha e^{-t \int_0^1 V(\gamma) ds} \left(\Xi_0 F(y), e^{-i\phi_0(\hat{\mathcal{K}})} \Xi_{\hbar ct} G(x) \right)_{\mathcal{F}_0} p_{\hbar^2 t}(x - y) \tag{5.1}$$

where $p_t(x) := e^{-|x|^2/(2t)} / \sqrt{(2\pi t)^d}$ and

$$\hat{\mathcal{K}} := \frac{e}{\sqrt{\hbar c}} \oplus_{\mu=1}^d \left(\sqrt{\hbar^2 t} \int_0^1 \xi_{\hbar ct s} \lambda(\cdot - \gamma) d\alpha_\mu(s) + (x_\mu - y_\mu) \int_0^1 \xi_{\hbar ct s} \lambda(\cdot - \gamma) ds \right)$$

where $\gamma = \gamma(x, y) := (1 - s)x + sy + \sqrt{\hbar^2 t} \alpha(s)$.

Proof. See appendix. □

Fix $t \geq 0$. Let $\Phi, \Psi \in \mathcal{F}$. For a bounded operator X on \mathcal{H} , we define a bilinear form $B_{\Psi, \Phi}(f, g)$ on $L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$ by

$$B_{\Psi, \Phi}(f, g) := (f \otimes \Psi, X(g \otimes \Phi))_{\mathcal{H}}.$$

Since

$$|B_{\Psi, \Phi}(f, g)| \leq \|\Psi\| \|\Phi\| \|f\| \|g\| \|X\|$$

there exists a bounded operator, $X_{\Psi, \Phi}$, on $L^2(\mathbb{R}^d)$ such that

$$B_{\Psi, \Phi}(f, g) = (f, X_{\Psi, \Phi}g)_{L^2(\mathbb{R}^d)}.$$

Let $\mathbb{B}(\mathcal{K})$ be the set of bounded operators on \mathcal{K} . Define

$$P_{\Psi, \Phi} : \mathbb{B}(\mathcal{H}) \rightarrow \mathbb{B}(L^2(\mathbb{R}^d))$$

by

$$P_{\Psi, \Phi}X := X_{\Psi, \Phi}.$$

Definition 5.5. Let $\Psi, \Phi \in \mathcal{F}$ and $X \in \mathbb{B}(\mathcal{H})$. Then we define $\text{Tr}_{\Psi, \Phi}(X)$ by

$$\text{Tr}_{\Psi, \Phi}(X) := \text{Tr}(P_{\Psi, \Phi}X) \quad \text{Tr}_{\Psi}(X) := \text{Tr}_{\Psi, \Psi}(X). \tag{5.2}$$

From (5.1) it is immediately seen that $P_{\Psi, \Phi}e^{-tH}$ is an integral operator such that, for $f, g \in L^2(\mathbb{R}^d)$,

$$(f, (P_{\Psi, \Phi}e^{-tH})g)_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} \overline{f(y)} K_{\Psi, \Phi}(x, y) g(x) dx dy \tag{5.3}$$

where

$$K_{\Psi, \Phi}(x, y) := \int_B d\alpha e^{-t \int_0^1 V(\gamma) ds} \left(\Xi_0 \Psi, e^{-i\phi_0(\hat{\kappa})} \Xi_{\hbar ct} \Phi \right) p_{\hbar^2 t}(y - x).$$

Definition 5.6. Let $\Psi, \Phi \in \mathcal{F}$. Then we define

$$\mathbf{K}_{\Psi, \Phi} := \int_{\mathbb{R}^d} K_{\Psi, \Phi}(x, x) dx = \frac{1}{\sqrt{(2\pi\hbar^2 t)^d}} \int_{\mathbb{R}^d \times B} dx d\alpha e^{-t \int_0^1 V(\hat{\gamma}) ds} \left(\Xi_0 \Psi, e^{-i\phi_0(\mathcal{Z})} \Xi_{\hbar ct} \Phi \right)$$

$$\mathbf{K}_{\Psi} := \mathbf{K}_{\Psi, \Psi}$$

where

$$\hat{\gamma} := \gamma(x, x) = x + \sqrt{\hbar^2 t} \alpha(s)$$

and

$$\mathcal{Z} := \frac{e\sqrt{\hbar t}}{\sqrt{c}} \oplus_{\mu=1}^d \int_0^1 \xi_s \lambda(\cdot - \gamma(x, x)) d\alpha_{\mu}(s).$$

Let

$$\text{Tr}_{\text{cl}}(e^{-t(p^2/2+V(x))}) := (2\pi\hbar)^{-d} \int_{\mathbb{R}^{2d}} e^{-t(p^2/2+V(x))} dp dx.$$

Lemma 5.7. Let $\Psi, \Phi \in \mathcal{F}$. We assume that V is continuous with $e^{-tV} \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$. Then $\lim_{\hbar \rightarrow 0} \mathbf{K}_{\Psi, \Phi} / \text{Tr}_{\text{cl}}(e^{-t(p^2/2+V(x))}) = (\Psi, \Phi)_{\mathcal{F}}$.

Proof. Set $F(\alpha) := e^{-t \int_0^1 V(\hat{\gamma}) ds} \left(\Xi_0 \Psi, e^{-i\phi_0(\mathcal{Z})} \Xi_{\hbar ct} \Phi \right)_{\mathcal{F}_0}$ and $\theta := (\Psi, \Phi)$. It suffices to show that

$$\lim_{\hbar \rightarrow 0} (2\pi\hbar^2 t)^{d/2} \mathbf{K}_{\Psi, \Phi} = \lim_{\hbar \rightarrow 0} \int_{\mathbb{R}^d} dx E_{\alpha}(F(\alpha)) = \int_{\mathbb{R}^d} dx e^{-tV(x)} \theta. \tag{5.4}$$

Note that, for Y -valued functions f_1, \dots, f_d on \mathbb{R}^d , it follows that [27, p 159]

$$\left(E_{\alpha} \left\| \int_0^1 f_{\mu}(\alpha(s)) d\alpha_{\mu}(s) \right\|_Y^2 \right)^{1/2} \leq \int_0^1 (E_{\alpha} \|f_{\mu}(\alpha(s))\|_Y^2)^{1/2} ds$$

$$+ \int_0^1 \frac{(E_{\alpha} \|\alpha_{\mu}(s) f_{\mu}(\alpha(s))\|_Y^2)^{1/2}}{1-s} ds. \tag{5.5}$$

Note that

$$\|\phi_0(f)\|_{\mathcal{F}_0}^2 \leq (\beta^2/2)\|f\|_Y^2.$$

Thus we have

$$(E_\alpha \|\phi_0(\mathcal{Z})\|_{\mathcal{F}_0}^2)^{1/2} \leq d e \beta \frac{\sqrt{\hbar t}}{\sqrt{c}} \|\lambda\| \left(1 + \sqrt{d} \int_0^1 \sqrt{\frac{s}{1-s}} ds\right).$$

Then it follows that

$$\lim_{\hbar \rightarrow 0} E_\alpha (\|\phi_0(\mathcal{Z})\|_{\mathcal{F}_0}^2) = 0$$

which implies that

$$\lim_{\hbar \rightarrow 0} (F, e^{-i\phi_0(\mathcal{Z})} G) = (F, G). \tag{5.6}$$

Let $\chi_R := \chi_{\{\alpha \in B \mid \|\alpha\|_\infty < R\}}$ and $\chi_{R^c} := \chi_{\{\alpha \in B \mid \|\alpha\|_\infty > R\}}$. For $K > 0$ and $R > 0$, we have

$$\left| \int_{\mathbb{R}^d} dx E_\alpha(F(\alpha)) - \int_{\mathbb{R}^d} dx e^{-tV(x)} \theta \right| \leq \left| \int_{\mathbb{R}^d} dx E_\alpha(F(\alpha) \chi_{R^c}) \right| \tag{5.7}$$

$$+ \left| \int_{|x| < K} dx E_\alpha(F(\alpha) \chi_R) - \int_{|x| < K} dx e^{-tV(x)} \theta E_\alpha(\chi_R) \right| \tag{5.8}$$

$$+ \left| \int_{|x| > K} dx E_\alpha(F(\alpha) \chi_R) \right| \tag{5.9}$$

$$+ \left| \int_{|x| < K} dx e^{-tV(x)} E_\alpha(\chi_{R^c}) + \int_{|x| > K} dx e^{-tV(x)} \right| \|\Psi\| \|\Phi\|. \tag{5.10}$$

It is known [27, p 166] that

$$\lim_{\hbar \rightarrow 0} (5.7) \leq \int_{\mathbb{R}^d} dx e^{-tV(x)} (1 - E_\alpha(\chi_R)) |\theta|$$

and it is easily seen that

$$\lim_{\hbar \rightarrow 0} (5.9) \leq \left| \int_{\mathbb{R}^d} dx e^{-tV(x)} - E_\alpha(\chi_R) \int_{|x| < K} dx e^{-tV(x)} \right| |\theta|.$$

While we see that, by (5.6) and the fact that Ξ_s is strongly continuous in s ,

$$\begin{aligned} \lim_{\hbar \rightarrow 0} (5.8) &= \lim_{\hbar \rightarrow 0} \int_{|x| < K} dx \int_{\|\alpha\|_\infty < R} d\alpha \left(e^{-t \int_0^t V(\hat{\gamma}) ds} - e^{-tV(x)} \right) (\Xi_0 \Psi, e^{-i\phi_0(\mathcal{Z})} \Xi_{\hbar ct} \Phi) \\ &+ \lim_{\hbar \rightarrow 0} \int_{|x| < K} dx \int_{\|\alpha\|_\infty < R} d\alpha e^{-tV(x)} (\Xi_0 \Psi, (e^{-i\phi_0(\mathcal{Z})} - 1) \Xi_{\hbar ct} \Phi) \\ &+ \lim_{\hbar \rightarrow 0} \int_{|x| < K} dx \int_{\|\alpha\|_\infty < R} d\alpha e^{-tV(x)} (\Xi_0 \Psi, (\Xi_{\hbar ct} - \Xi_0) \Phi) \\ &\leq \lim_{\hbar \rightarrow 0} \int_{|x| < K} dx \int_{\|\alpha\|_\infty < R} d\alpha \left| e^{-t \int_0^t V(\hat{\gamma}) ds} - e^{-tV(x)} \right| \|\Psi\| \|\Phi\| \\ &+ \|e^{-tV}\|_\infty \lim_{\hbar \rightarrow 0} \int_{|x| < K} dx \int_{\|\alpha\|_\infty < R} d\alpha |(\Xi_0 \Psi, (e^{-i\phi_0(\mathcal{Z})} - 1) \Xi_{\hbar ct} \Phi)| \\ &+ \|e^{-tV}\|_\infty \lim_{\hbar \rightarrow 0} \int_{|x| < K} dx \int_{\|\alpha\|_\infty < R} d\alpha e^{-tV(x)} |(\Xi_0 \Psi, (\Xi_{\hbar ct} - \Xi_0) \Phi)| = 0. \end{aligned}$$

Hence, for arbitrary $\epsilon > 0$, taking sufficiently large R and K , we have

$$\lim_{\hbar \rightarrow 0} \{(5.7) + (5.8) + (5.9) + (5.10)\} < \epsilon.$$

Thus the lemma follows. \square

We shall give a sufficient condition so that $P_{\Psi, \Phi} e^{-tH}$ is of trace class.

Lemma 5.8. *Let $\Psi, \Phi \in \mathcal{F}$. Let V be continuous with $e^{-tV} \in L^\infty(\mathbb{R}^d)$. Then $K_{\Psi, \Phi}(x, y)$ is continuous in $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$.*

Proof. Set $\hat{K}' := \hat{K}(x', y')$, First we shall prove that

$$s - \lim_{(x', y') \rightarrow (x, y)} e^{-i\phi_0(\hat{K}')} F = e^{-i\phi_0(\hat{K})} F \quad F \in \mathcal{F}_0 \quad (5.11)$$

in $L^2(B; \mathcal{F}_0)$. Set

$$\begin{aligned} \Gamma_\mu &:= \Gamma_\mu(x, y) := \bigoplus_{\nu=1}^d \delta_{\mu\nu} \lambda(\cdot - \gamma(x, y)) \\ \Gamma'_\mu &:= \Gamma_\mu(x', y') \quad \delta_\mu := y_\mu - x_\mu \quad \delta'_\mu := y'_\mu - x'_\mu. \end{aligned}$$

We have, by (5.5)

$$\begin{aligned} (E_\alpha \|\phi_0(\hat{K}') - \phi_0(\hat{K})\|_{\mathcal{F}_0}^2)^{1/2} &\leq \beta e^{\frac{\sqrt{2\hbar}t}{\sqrt{c}}} \sum_{\mu=1}^d \int_0^1 (E_\alpha \|\Gamma_\mu - \Gamma'_\mu\|_W^2)^{1/2} ds \\ &+ \beta e^{\frac{\sqrt{2}}{\sqrt{\hbar}c}} \sum_{\mu=1}^d \int_0^1 ds \left\{ \frac{(\hbar^2 t E_\alpha \alpha(s)^2 \|\Gamma_\mu - \Gamma'_\mu\|_W^2)^{1/2}}{1-s} \right. \\ &\left. + (E_\alpha \|\Gamma_\mu \delta_\mu - \Gamma'_\mu \delta'_\mu\|_W^2)^{1/2} \right\}. \end{aligned} \quad (5.12)$$

Since it is seen that

$$\|\Gamma_\mu - \Gamma'_\mu\|_W^2 = \int_{\mathbb{R}^d} |\hat{\lambda}(k)|^2 \left| e^{i(1-s)xk + isy'k} - e^{i(1-s)x'k + isy'k} \right|^2 dk$$

we have

$$\lim_{(x', y') \rightarrow (x, y)} \|\Gamma_\mu - \Gamma'_\mu\|_W^2 = 0.$$

Thus each term in (5.12) goes to zero as $(x', y') \rightarrow (x, y)$. Hence we have

$$E_\alpha \left(\|\phi_0(\hat{K}') - \phi_0(\hat{K})\|_{\mathcal{F}_0}^2 \right) \rightarrow 0$$

as $(x', y') \rightarrow (x, y)$, which yields (5.11). Since

$$\begin{aligned} &K_{\Psi, \Phi}(x', y') - K_{\Psi, \Phi}(x, y) \\ &= E_\alpha \left\{ e^{-t \int_0^1 V(\gamma) ds} p_{\hbar^2 t}(y-x) \left(\Xi_0 \Psi, \left(e^{-i\phi_0(\hat{K}')} - e^{-i\phi_0(\hat{K})} \right) \Xi_{\hbar ct} \Phi \right) \right\} \\ &+ E_\alpha \left\{ \left(\Xi_0 \Psi, e^{-i\phi_0(\hat{K}')} \Xi_{\hbar ct} \Phi \right) \right. \\ &\left. \times \left(e^{-t \int_0^1 V(\gamma') ds} p_{\hbar^2 t}(y'-x') - e^{-t \int_0^1 V(\gamma) ds} p_{\hbar^2 t}(y-x) \right) \right\} \end{aligned} \quad (5.13)$$

the Lebesgue-dominated convergence theorem and (5.11) yield that the right-hand side of (5.13) converges to zero as $(x', y') \rightarrow (x, y)$. \square

Lemma 5.9. *Let $\Psi \in \mathcal{F}$. Let V be continuous with $e^{-tV} \in L^\infty(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$. Then $P_{\Psi,\Psi}e^{-tH}$ is a trace class and $\text{Tr}_\Psi(e^{-tH}) = \mathbf{K}_\Psi$.*

Proof. $K_{\Psi,\Psi}(x, y)$ is continuous by lemma 5.8 and positive definite, i.e.,

$$\int_{\mathbb{R}^{2d}} \overline{f(x)} K_{\Psi,\Psi}(x, y) f(y) dx dy = (f \otimes \Psi, e^{-tH} f \otimes \Psi) \geq 0 \quad f \in L^2(\mathbb{R}^d).$$

By Jensen’s inequality, we have

$$\frac{|\mathbf{K}_{\Psi,\Psi}|}{\|\Psi\| \|\Phi\|} \leq \frac{1}{\sqrt{(2\pi\hbar^2 t)^d}} \int_{\mathbb{R}^d} dx \int_B d\alpha \int_0^1 ds e^{-tV(\hat{y})} = \text{Tr}_{\text{cl}}(e^{-t(p^2/2+V(x))}).$$

Hence we have

$$\left| \int_{\mathbb{R}^d} K_{\Psi,\Psi}(x, x) dx \right| \leq \text{Tr}_{\text{cl}}(e^{-t(p^2/2+V(x))}) \|\Psi\|^2 < \infty.$$

Then by [25, p 65] and [28, theorem 2.12], $\text{Tr}_\Psi(e^{-tH}) = \int_{\mathbb{R}^d} K_{\Psi,\Psi}(x, x) dx = \mathbf{K}_\Psi$. Thus the lemma follows. \square

Theorem 5.10. *We assume the same conditions as those of lemma 5.9. Then*

$$\lim_{\hbar \rightarrow 0} \text{Tr}_\Psi(e^{-tH}) / \text{Tr}_{\text{cl}}(e^{-t(p^2/2+V(x))}) = \|\Psi\|^2.$$

Proof. It follows from lemmas 5.7 and 5.9. \square

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Appendix

A proof of Lemma 5.4. Generally, for measurable functions f, h , and g_1, \dots, g_d on \mathbb{R}^d ,

$$\int_M h(X) f \left(\sum_{\mu=1}^d \int_0^t g_\mu(X_s) db_\mu(s) \right) dX = \int_{\mathbb{R}^{2d} \times B} h(\gamma) f(Q) p_t(x - y) dx dy d\alpha \quad (6.1)$$

where

$$Q := \sqrt{t} \sum_{\mu=1}^d \int_0^1 g_\mu(\gamma) d\alpha_\mu(s) + \sum_{\mu=1}^d (x_\mu - y_\mu) \int_0^1 g_\mu(\gamma) ds.$$

We denote by $\langle \phi_0, f \rangle \in \mathbb{R}$ the value of $\phi_0(f)$ at $\phi_0 \in Q_0$. Since

$$\int_0^t \phi_0(\xi_s \lambda_\mu(X_s)) db_\mu(s) = s - \lim_{n \rightarrow \infty} \sum_{k=1}^{2^n} \phi_0(\xi_{\Delta_k} \lambda_\mu(X_{\Delta_k})) (b_\mu(\Delta_{k+1}) - b_\mu(\Delta_k))$$

in $L^2(M; \mathcal{F}) \cong L^2(Q; L^2(M))$, there exists $\mathbf{Q} \subset Q_0$ with $\int_{\mathbf{Q}} d\mu_0 = 1$ such that, taking a subsequence, $\{n'\}$, we have

$$\left(\int_0^t \phi_0(\xi_s \lambda_\mu(X_s)) db_\mu(s) \right) (\phi_0) = s - \lim_{n' \rightarrow \infty} \sum_{k=1}^{2^{n'}} \langle \phi_0, \xi_{\Delta_k} \lambda_\mu(X_{\Delta_k}) \rangle (b_\mu(\Delta_{k+1}) - b_\mu(\Delta_k))$$

in $L^2(M)$ for $\phi_0 \in \mathbf{Q}$. Then

$$\left(\int_0^t \phi_0(\xi_s \lambda_\mu(X_s)) db_\mu(s) \right) (\phi_0) = \int_0^t \langle \phi_0, \xi_s \lambda_\mu(X_s) \rangle db_\mu(s) \quad (6.2)$$

for $\phi_0 \in \mathbf{Q}$ in $L^2(M, dX)$. Note that the right-hand side of (6.2) is a stochastic integral of real-valued function $\langle \phi_0, \xi_s \lambda_\mu(X_s) \rangle$, but the left-hand side is the value of \mathcal{F}_0 -valued stochastic integral $\int_0^t \phi_0(\xi_s \lambda_\mu(X_s)) db_\mu(s)$ at $\phi_0 \in Q_0$. While, in the same manner as (6.2), it follows that there exists $\hat{\mathbf{Q}} \subset Q_0$ such that $\int_{\hat{\mathbf{Q}}} d\mu_0 = 1$ and that

$$\left(\int_0^1 \phi_0(\xi_s \lambda_\mu(\gamma)) d\alpha_\mu(s) \right) (\phi_0) = \int_0^1 \langle \phi_0, \xi_s \lambda_\mu(\gamma) \rangle d\alpha_\mu(s) \quad (6.3)$$

for $\phi_0 \in \hat{\mathbf{Q}}$ in $L^2(B, d\alpha)$. Let $F = f \otimes \Psi$ and $G = g \otimes \Phi$. For each $\phi_0 \in \mathbf{Q} \cap \hat{\mathbf{Q}}$, by (6.1), we see that

$$\begin{aligned} & \int_M \overline{f(X_0)} g(X_t) \exp\left(-\int_0^t V(X_s) ds\right) \exp\left(-i e \sum_{\mu=1}^d \int_0^t \langle \phi_0, \xi_s \lambda_\mu(X_s) \rangle db_\mu(s)\right) \\ &= \int_{\mathbb{R}^{2d}} dx dy p_t(x-y) \overline{f(x)} g(y) \int_B d\alpha \exp\left(-t \int_0^1 V(\gamma) ds\right) \\ & \times \exp\left(-i e \sum_{\mu=1}^d \left(\sqrt{t} \int_0^1 \langle \phi_0, \xi_s \lambda_\mu(\gamma) \rangle d\alpha_\mu(s) + (x_\mu - y_\mu) \int_0^1 \langle \phi_0, \xi_s \lambda_\mu(\gamma) \rangle ds\right)\right). \end{aligned}$$

Hence from (2.3), (6.2) and (6.3), (5.1) follows. \square

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