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General quantum surface-of-section method

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Abstract. A new method for *exact* quantization of general bound Hamiltonian systems is presented. It is the quantum analogue of the classical Poincaré surface-of-section (SOS) reduction of classical dynamics. The quantum Poincaré mapping is shown to be the product of the two *generalized* (*non-unitary* but *compact*) on-shell scattering operators of the two scattering Hamiltonians which are obtained from the original bound one by cutting the f-dimensional configuration space (CS) the along the $(f-1)$-dimensional configurational SOS and attaching the flat quasi-one-dimensional waveguides instead. The quantum Poincaré mapping has fixed points at the eigenenergies of the original bound Hamiltonian. The energy-dependent quantum propagator $(E-\hat{H})^{-1}$ can be decomposed in terms of the four energy-dependent propagators which propagate from and/or to CS to and/or from configurational SOS (which may generally be composed of many disconnected parts).

I show that in the semiclassical limit ($\hbar \to 0$) the quantum Poincaré mapping converges to the Bogomolny's propagator and explain how the higher-order semiclassical corrections can be obtained systematically.

1. Introduction

Over the last decade or two there has been an increasing interest in efficient quantization procedures for simple (having only few freedoms) but nonlinear (possibly chaotic) Hamiltonian systems. Here I consider *bound* and *autonomous* Hamiltonian systems with f freedoms. Directly solving the time-independent Schrödinger equation in f-dimensional configuration space (CS) or the equivalent eigenvalue problem for the Hamiltonian matrix in an appropriate basis is the first but certainly not the best idea. A question was raised in [7] as to whether there exists a quantum analogue of the surface-of-section (SOS) reduction of classical dynamics [5] which reduces smooth bound and autonomous Hamiltonian dynamics over $2f$-dimensional phase space to a discrete Poincaré mapping over only $(2f-2)$-dimensional SOS.

In the case of quantum billiard systems in two dimensions ($f=2$) we have the so-called boundary integral method which reduces a two-dimensional Schrödinger equation to a one-dimensional integral equation. Its kernel can be interpreted as the quantum bounce map which is a special case of Poincaré mapping. Smilansky and coworkers [2, 14] have developed a more general *scattering approach for quantization of billiards*. They construct exact quantum Poincaré mapping for two-dimensional billiards with respect to the arbitrary line of section as the product of the two scattering matrices of the two opened billiards. These methods are typically much more efficient than the direct diagonalization, since the

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dimension of the matrices they use is typically of the order of the square root of the dimension of the original Hamiltonian matrix. On the other hand Bogomolny succeeded in constructing an approximate semiclassical Poincaré mapping with respect to an arbitrary configurational surface of section for an arbitrary autonomous Hamiltonian. In this paper I present the generalization of the scattering approach for quantization of almost arbitrary bound Hamiltonians and show that it reduces to the Bogomolny's theory in the semiclassical limit $\hbar \to 0$.

In section 2 I construct the quantum Poincaré mapping and prove that the eigenenergies of the original Hamiltonian correspond to the fixed points of quantum Poincaré mapping. I also prove theoretically a perhaps even more interesting SOS decomposition of the resolvent of the Hamiltonian. Here I also study the semiclassical limit of newly defined propagators and explicitly calculate the leading-order and next-to-leading order terms while I explain how higher-order corrections (in powers of $\hbar$) can be obtained systematically. The symmetries of quantum Poincaré mapping are discussed and it is explained how the SOS quantization condition can be used very efficiently in practical calculations, especially for the generic class of the so-called *semi-separable systems*. In section 3 I formulate an abstract quantum SOS method which can be applied to *arbitrary boundary-value differential equation* problems. Then I apply an abstract theory to the case of the energy-dependent Schrödinger equation of section 2 and more general cases of non-relativistic or even relativistic systems (described by the Dirac equation) coupled to arbitrary external gauge fields. In section 4 the method is generalized to the case of non-simply but multiply-connected CSOS. In section 5 I discuss the meaning and applicability of the new results and reach conclusions. Some preliminary results of this project have already been reported [9, 10].

The idea behind the proofs of the major results, although they are technically quite complex, is very simple. We assume that a bounded energy-dependent (stationary) Schrödinger equation with the prescribed values of the wavefunction on $(f-1)$-dimensional configurational SOS has unique solutions on both sides of CS with respect to the configurational SOS. Then we study the (quantization) conditions under which these two solutions may be matched smoothly to give an eigenfunction over the entire CS, such that it is continuous and continuously differentiable on the configurational SOS. I have tried to argue in an intuitive physical way as much as possible, however, the use of some technical mathematical tools and formulations is unavoidable. Nevertheless, the results are believed and shown to be correct on intuitive physical grounds but the proofs are not yet fully rigorous.

2. Surface-of-section quantization

2.1. Notation

The basic results of this paper are most beautifully and compactly written in terms of some new physical quantities whose mathematical definitions and notation are described in this subsection.

We study *autonomous* and *bound* (at least in the energy region of our concern) Hamiltonian systems with few, say f, freedoms, living in an f-dimensional *configuration space (CS) $\mathcal{C}$. One should also provide a smooth $(f-1)$-dimensional submanifold* of CS $\mathcal{C}$ which shall be called the *configurational surface of section* (CSOS)† and denoted by $\mathcal{S}_0$.

† The more general case of a $(2f-2)$-dimensional SOS in a $2f$-dimensional phase space which is not perpendicular to CS cannot be treated within the present approach except in the cases where one can change the phase space coordinates by means of an appropriate canonical transformation.

In this section we only consider the case of *simply-connected* CSOS whereas in section 4 we study the case of more general *multiply-connected* CSOS. We choose the coordinates in CS, $q = (x, y) \in \mathcal{C}$ in such a way that the CSOS is given by a simple constraint $y = 0$, or $\mathcal{S}_0 = (\mathcal{S}, 0)$. These coordinates *need not be global*, i.e. they need not cover the whole CS, but they should cover the open set which includes the whole CSOS $\mathcal{S}_0$. This means that every point in $\mathcal{S}_0$ should be uniquely represented by CSOS coordinates $x \in \mathcal{S}$ which *may be more general* than Euclidean coordinates $\mathcal{R}^{f-1}$ (e.g. $(f-1)$-dim sphere S^{f-1}). In this section we shall assume that $\mathcal{S}_0$ is an *orientable manifold* so that it cuts the CS $\mathcal{C}$ in two pieces which will be referred to as upper and lower and denoted by the value of the binary index $\sigma = \uparrow, \downarrow$ (see figure 1). In arithmetic expressions the arrows will have the following values $\uparrow = +1, \downarrow = -1$. My approach presented in this section applies to a quite general class of bound Hamiltonians whose kinetic energy is quadratic, at least perpendicularly to CSOS,

$$H = \frac{1}{2m} p_y^2 + H'(p_x, x, y). \tag{1}$$

In the following sections we generalize this class to include Hamiltonians having coordinate-dependent mass (which arise in the *curvilinear coordinates which must be used in the case of non-flat CSOS*) and/or terms linear in p_y (which appear, for example, due to the *presence of a magnetic field*).

In quantum mechanics, the observables are represented by self-adjoint operators in a Hilbert space $\mathcal{H}$ of complex-valued functions $\Psi(q)$ over the CS $\mathcal{C}$ which obey boundary conditions $\Psi(\partial\mathcal{C}) = 0$ and have a finite L^2-norm $\int_{\mathcal{C}} \mathrm{d}q\, |\Psi(q)|^2 < \infty$. We shall use the Dirac notation. A pure state of a physical system is represented by a vector (ket$|\Psi\rangle$) which can be expanded in a convenient complete set of basis vectors, e.g. position eigenvectors $|q\rangle = |x, y\rangle$, $|\Psi\rangle = \int_{\mathcal{C}} \mathrm{d}q\, |q\rangle\langle q|\Psi\rangle = \int_{\mathcal{C}} \mathrm{d}q\, \Psi(q)|q\rangle$ (in a symbolic sense, since $|q\rangle$ are not proper vectors, but such expansions are still meaningful iff $\Psi(q) = \langle q|\Psi\rangle$ is square

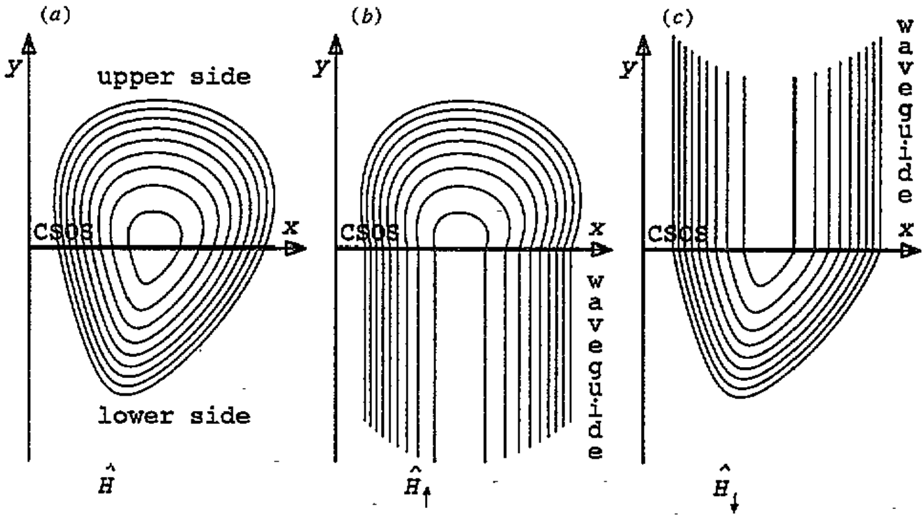

Figure 1. The geometry of the two-dimensional CS of a typical bound system, (*a*) with simply connected CSOS. Isopotential contours are shown. The product of classical or quantal scattering mappings of the two scattering systems shown in (*b*) and (*c*) is equal to the classical or quantal Poincaré mapping of a bound system (*a*).

integrable i.e. a $L^2(\mathcal{C})$-function). Every ket $|\Psi\rangle \in \mathcal{H}$ has a corresponding vector from the dual Hilbert space $\mathcal{H}'$, that is bra $\langle\Psi| \in \mathcal{H}'$, $\langle\Psi|q\rangle = \langle q|\Psi\rangle^*$. We shall the use mathematical accent $\hat{}$ to denote linear operators over the Hilbert space $\mathcal{H}$. Operators of SOS coordinates $\hat{x}$ and $\hat{p}_x$, defined by†

$$\langle x, y|\hat{x}|\Psi\rangle = x\Psi(x, y) \qquad \langle x, y|\hat{p}_x|\Psi\rangle = -i\hbar\partial_x\Psi(x, y)$$

can also be viewed as acting on functions $\psi(x)$ of x only and therefore operating in some other, much smaller Hilbert space of square-integrable complex-valued functions over a CSOS $\mathcal{S}_0$

$$\{x|\check{x}|\psi\} = x\psi(x) \qquad \{x|\check{p}_x|\psi\} = -i\hbar\partial_x\psi(x).$$

Vectors in such a reduced SOS-Hilbert space, denoted by $\mathcal{L}$, will be written as $|\psi\}$ and linear operators over $\mathcal{L}$ will have a mathematical accent $\check{}$ like the restricted position $\check{x}$ and momentum $\check{p}_x$. Eigenvectors $|x\}$ of the SOS-position operator $\check{x}$ provide a useful complete set of basis vectors of $\mathcal{L}$. The quantum Hamiltonian can be written as

$$\hat{H} = -\frac{\hbar^2}{2m}\partial_y^2 + \hat{H}'(y) \qquad \hat{H}'(y) = H'(-i\hbar\partial_x, x, y). \tag{2}$$

The eigenstates of the reduced *inside-CSOS Hamiltonian* $\check{H}'(0) = \hat{H}'(0)|_{\mathcal{L}}$ restricted to the SOS-Hilbert space $\mathcal{L}$, $|n\} \in \mathcal{L}$

$$\check{H}'(0)|n\} = E'_n|n\} \tag{3}$$

which are called *SOS-eigenmodes*, provide a useful (countable $n = 1, 2, \ldots$) complete and orthogonal basis for $\mathcal{L}$ since $\check{H}'(0)$ is a self-adjoint operator with discrete spectrum when its domain is restricted to $\mathcal{L}$.

The major problem of bound quantum dynamics is to determine the *eigenenergies* E for which the *Schrödinger equation*

$$\langle x, y|\hat{H}|\Psi(E)\rangle = E\Psi(x, y, E) \tag{4}$$

has non-trivial normalizable solutions—*eigenfunctions* $\Psi(x, y, E)$.

2.2. Scattering formulation

In this subsection I will introduce our basic tools using the powerful quantum mechanical time-independent multichannel scattering theory [8, 15].

To connect bound Hamiltonian dynamics and scattering theory one should make the following very important step. Cut one part of CS off along CSOS and attach a semi-infinite separable (flat along the y-axis) waveguide instead (see figure 1). Thus we introduce two scattering Hamiltonians

$$\hat{H}_\sigma = \begin{cases} -(\hbar^2/2m)\partial_y^2 + \hat{H}'(y) & \sigma y \geqslant 0 \\ -(\hbar^2/2m)\partial_y^2 + \hat{H}'(0) & \sigma y < 0. \end{cases} \tag{5}$$

Every wavefunction inside the waveguide ($\sigma y \leqslant 0$) at energy E can be separated as the superposition of products of a bound state (SOS-eigenmode n) in the x-direction and free motion in the y-direction,

$$\{x|n\}\, e^{\pm i k_n(E) y}$$

† In the case of the non-Euclidean SOS they should be replaced by the generators of the corresponding Lie algebra.

with the corresponding wavenumber determined by the energy difference $E - E'_n$ available for the motion perpendicular to the CSOS

$$k_n(E) = \sqrt{\frac{2m}{\hbar^2}(E - E'_n)}\,.$$

For any value of energy E, there is typically a finite number of the so-called open or propagating SOS-eigenmodes—channels with real wavenumbers for which $E'_n < E$, and infinitely many closed channels with imaginary wavenumbers for which $E'_n > E$. The scattering wavefunction $\Psi_\sigma(x, y, E)$ at a given energy E (or complex-conjugated wavefunction $\Psi^*_\sigma(x, y, E^*) = (\Psi_\sigma(x, y, E^*))^*$) satisfying the Schrödinger equation $\hat{H}_\sigma|\Psi_\sigma(E)\rangle = E|\Psi_\sigma(E)\rangle$ can be uniquely parametrized by the vector $|\psi\}$ from the SOS-Hilbert space $\mathcal{L}$ (or by vector $\{\psi^*|$ from the dual SOS-Hilbert space $\mathcal{L}'$). $|\psi\} \in \mathcal{L}$ essentially parametrize the incoming waves

$$\Psi^{\mathrm{in}}_\sigma(x, y, E) = \sum_n \{x|n\}\sqrt{\frac{m}{\mathrm{i}\hbar^2 k_n(E)}}\,\mathrm{e}^{\mathrm{i}\sigma k_n(E)y}\{n|\psi\}$$

which uniquely determine the whole scattering wavefunction. Therefore the *wave operators* can be defined, namely $\acute{Q}'_\sigma(E)$ which map from $\mathcal{L}$ to $\mathcal{H}$ (or $\grave{P}'_\sigma(E)$ which map from $\mathcal{H}$ to $\mathcal{L}$) and whose kernels are given by the scattering wavefunctions (or their complex conjugates)

$$\langle q|\acute{Q}'_\sigma(E)|\psi\} = \Psi_\sigma(q, E) \tag{6}$$

$$\{\psi^*|\grave{P}'_\sigma(E)|q\rangle = \Psi^*_\sigma(q, E^*)\,. \tag{7}$$

On the σ-side of CS ($\sigma y \geqslant 0$) the scattering wavefunction *satisfies the ordinary Schrödinger equation* (4) whereas in the waveguide ($\sigma y \leqslant 0$) it is a superposition of incoming and scattered waves

$$\begin{aligned}\Psi_\sigma(x, y, E) &= \frac{\sqrt{-\mathrm{i}m}}{\hbar}\sum_{n,l}\{x|n\}k_n^{-1/2}(E)\left[\mathrm{e}^{\mathrm{i}\sigma k_n(E)y}\delta_{nl} + \mathrm{e}^{-\mathrm{i}\sigma k_n(E)y}T^\sigma_{nl}\right]\{l|\psi\} \\ &= \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{x|\check{K}^{-1/2}(E)\left[\mathrm{e}^{\mathrm{i}\sigma\check{K}(E)y} + \mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y}\check{T}_\sigma(E)\right]|\psi\}\end{aligned} \tag{8}$$

$$\Psi^*_\sigma(x, y, E^*) = \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{\psi^*|\left[\mathrm{e}^{\mathrm{i}\sigma\check{K}(E)y} + \check{T}_\sigma(E)\,\mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y}\right]\check{K}^{-1/2}(E)|x\}\,. \tag{9}$$

For the sake of compact notation we have introduced the *wavenumber operator*

$$\check{K}(E) = \sum_n k_n(E)|n\}\{n| = \sqrt{\frac{2m}{\hbar^2}(E - \check{H}'(0))}\,. \tag{10}$$

$T^\sigma_{nl}(E)$ is the generalized *scattering matrix* since it also includes closed (non-propagating) modes and $\check{T}_\sigma(E)$ is the corresponding scattering operator over $\mathcal{L}$

$$\check{T}_\sigma(E) = \sum_{n,l} T^\sigma_{nl}|n\}\{l|\,. \tag{11}$$

Here I have to make three important notes:

- the conjugated energy E^* is used in the argument of the complex-conjugated wavefunction (7) in order to make all the relevant operators, e.g. $\grave{P}'_\sigma(E)$, complex analytic functions of E rather than E^*.
- The SOS-states $|\psi^*\}$ and $|\psi\}$ are generally different.

- The equation (9) is non-trivial and does not follow from (8) but it is a consequence of the *Hermitian* symmetry of the scattering Hamiltonians $\hat{H}_\sigma$ as will be shown in the next paragraph.

Let us now consider the resolvents of the scattering Hamiltonians (5) with outgoing boundary conditions

$$\hat{G}_\sigma(E) = \frac{1}{\mathrm{i}\hbar}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E-\hat{H}_\sigma)t/\hbar} = (E - \hat{H}_\sigma + \mathrm{i}0)^{-1}\,. \tag{12}$$

It is convenient to introduce a hybrid representation of these scattering Green functions denoted by $\check{G}_\sigma(y, y', E) \in \mathcal{L}$ (being a matrix element in the y-variable and an operator in the x-variable) defined as

$$\{x|\check{G}_\sigma(y, y', E)|x'\} = \langle x, y|\hat{G}_\sigma(E)|x', y'\rangle\,. \tag{13}$$

Inside the waveguide ($\sigma y \leqslant 0, \sigma y' \leqslant 0$) these hybrid Green functions satisfy the following 'free-motion' Schrödinger equations in both arguments:

$$\partial_y^2 \check{G}_\sigma(y, y', E) + \check{K}^2(E)\check{G}_\sigma(y, y', E) = \frac{2m}{\hbar^2}\delta(y - y') \tag{14}$$

$$\partial_{y'}^2 \check{G}_\sigma(y, y', E) + \check{G}_\sigma(y, y', E)\check{K}^2(E) = \frac{2m}{\hbar^2}\delta(y - y')\,. \tag{15}$$

The general solution of this linear system (in the waveguide) is given by the sum of *particular* 'free-motion' solution

$$\check{G}_{\text{free}}(y, y', E) = \frac{m}{\mathrm{i}\hbar^2}\check{K}^{-1/2}(E)\,\mathrm{e}^{\mathrm{i}\check{K}(E)|y-y'|}\check{K}^{-1/2}(E)$$

and general solution of the homogeneous system satisfying outgoing boundary conditions

$$\check{G}_\sigma(y, y', E) - \check{G}_{\text{free}}(y, y', E) = \frac{m}{\mathrm{i}\hbar^2}\check{K}^{-1/2}(E)\,\mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y}\check{A}\,\mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y'}\check{K}^{-1/2}(E)\,. \tag{16}$$

Their sum $\{x|\check{G}_\sigma(y, 0, E)$ satisfies the Schrödinger equation (4) on the σ-side ($\sigma y \geqslant 0$), so comparing it locally, at $\sigma y = +0$, with wavefunctions (8) yields

$$\Psi_\sigma(x, y, E) = \frac{\hbar}{\sqrt{-\mathrm{i}m}}\{x|\check{G}_\sigma(y, 0, E)\check{K}^{1/2}(E)|\psi\} \qquad \sigma y \geqslant 0 \tag{17}$$

and determines the free operator valued parameter, $\check{A} = \check{T}_\sigma(E)$. Thus the waveguide expression for the hybrid scattering Green function reads ($\sigma y \leqslant 0, \sigma y' \leqslant 0$)

$$\check{G}_\sigma(y, y', E) = \frac{m}{\mathrm{i}\hbar^2}\check{K}^{-1/2}(E)\left[\mathrm{e}^{\mathrm{i}\check{K}(E)|y-y'|} + \mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y}\check{T}_\sigma(E)\,\mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y'}\right]\check{K}^{-1/2}(E)\,. \tag{18}$$

Since $\check{G}_\sigma(0, y, E)|x\}$ satisfies conjugated Schrödinger equation, there exist SOS-states $|\psi^*\}$ such that

$$\Psi_\sigma^*(x, y, E^*) = \frac{\hbar}{\sqrt{-\mathrm{i}m}}\{\psi^*|\check{K}^{1/2}(E)\check{G}_\sigma(0, y, E)|x\} \qquad \sigma y \geqslant 0 \tag{19}$$

and equation (9) follows.

2.3. SOS energy quantization

Now I shall formulate an exact energy quantization condition for the original Hamiltonian matrix $\check{H}$ solely in terms of the scattering operators $\check{T}_\sigma(E)$.

Theorem 1a. Every energy E for which the operator $1 - \check{T}_\downarrow(E)\check{T}_\uparrow(E)$ (where the order of the arrows may be reversed) is singular is

- either eigenenergy of the original Hamiltonian $\hat{H}$,
- or it is a threshold energy for opening of a new channel,
- or both.

More precisely: the dimensions of the left and right null-space of an operator $1-\check{T}_\downarrow(E)\check{T}_\uparrow(E)$ are the same

$$d_T(E) = \dim\ker(1 - \check{T}_\downarrow(E)\check{T}_\uparrow(E)) = \dim\ker(1 - \check{T}_\downarrow(E)\check{T}_\uparrow(E))^\dagger \tag{20}$$

and the following inequality for $d_T(E)$ in terms of the dimension of the null space of operator $E-\hat{H}$, $d_H(E) = \dim\ker(E-\hat{H})$, and the dimension of the null space of operator $\check{K}^2(E)$, $d_K(E) = \dim\ker\check{K}^2(E)$, holds

$$\max\{d_H(E), d_K(E)\} \leqslant d_T(E) \leqslant d_H(E) + d_K(E)\,. \tag{21}$$

Proof. Let $d_T(E_0)$ SOS-states $|\uparrow n\} \in \mathcal{L}$, $n = 1, \ldots, d_T(E_0)$ span the null space of $1 - \check{T}_\downarrow(E_0)\check{T}_\uparrow(E_0)$

$$\left(1 - \check{T}_\downarrow(E_0)\check{T}_\uparrow(E_0)\right)|\uparrow n\} = 0\,. \tag{22}$$

Then one may define another set of $d_T(E_0)$ SOS states $|\downarrow n\} \in \mathcal{L}$ by the prescription

$$|\downarrow n\} = \check{T}_\uparrow(E_0)|\uparrow n\} \tag{23}$$

in terms of which the equation (22) may be rewritten as a relation symmetric to (23)

$$|\uparrow n\} = \check{T}_\downarrow(E_0)|\downarrow n\}\,. \tag{24}$$

Each of these vectors $|\uparrow n\}$ lies either in the null space or in the image of $\check{K}^2(E_0)$, since

$$\mathcal{L} = \ker\check{K}^2(E_0) \oplus \check{K}^2(E_0)\mathcal{L}$$

where $\check{K}^2(E)\mathcal{L} = \ker\check{K}^2(E)^\perp$ since $\check{K}^2(E)$ is self-adjoint. Let the first m_K vectors $|\uparrow m\}$, $m = 1, \ldots, m_K$ lie in $\ker\check{K}^2(E)$. In order to make sure that scattering wavefunctions (8) and (9) have a regular limit $E \to E_0$, since $\check{K}^{-1/2}(E)$ is becoming singular if $\ker\check{K}^2(E_0) \neq \emptyset$, one should demand

$$(1 + \check{T}_\sigma(E_0))|\phi\} = 0 \qquad \{\phi|(1 + \check{T}_\sigma(E_0)) = 0 \tag{25}$$

for any $|\phi\} \in \ker\check{K}^2(E_0)$, so $\ker\check{K}^2(E_0)$ is invariant under $\check{T}_\sigma(E_0)$ and $\check{T}_\sigma^\dagger(E_0)$

$$\check{T}_\sigma(E_0)\ker\check{K}^2(E_0) = \check{T}_\sigma^\dagger(E_0)\ker\check{K}^2(E_0) = \ker\check{K}^2(E_0)\,.$$

From equation (25) we also see that $\ker\check{K}^2(E_0) \subseteq \ker(1 - \check{T}_\downarrow(E_0)\check{T}_\uparrow(E_0))$, so $|\uparrow m\}$ span the entire space $\ker\check{K}^2(E_0)$, and so $d_K(E_0) = m_K \leqslant d_T(E_0)$. Therefore the image $\check{K}^2(E)\mathcal{L}$ is also invariant under $\check{T}_\sigma(E_0)$ and $\check{T}_\sigma^\dagger(E_0)$, so the counterparts $|\downarrow l\}$ of the remaining $d_T(E_0) - d_K(E_0)$ SOS-states $|\uparrow l\}$, $l = d_K(E_0) + 1, \ldots, d_T(E_0)$ from the image $\check{K}^2(E)\mathcal{L}$ also lie in the image $\check{K}^2(E)\mathcal{L}$. In the image one can define the inverse of $\check{K}^2(E_0)$ and the inverse of its fourth root, namely $\check{K}^{-1/2}(E_0)$. Using equations (23) and (24) one can write

$$\left(1 + \check{T}_\uparrow(E_0)\right)|\uparrow l\} = \left(1 + \check{T}_\downarrow(E_0)\right)|\downarrow l\}$$

$$\left(1 - \check{T}_\uparrow(E_0)\right)|\uparrow l\} = -\left(1 - \check{T}_\downarrow(E_0)\right)|\downarrow l\}$$

which can be rewritten using the values of the wavefunctions and their normal derivatives on the CSOS (from (8))

$$\langle x, 0|\acute{Q}'_\sigma(E)|\psi\} = \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{x|\check{K}^{-1/2}(E)\big(1+\check{T}_\sigma(E)\big)|\psi\} \tag{26}$$

$$\partial_y\langle x, y|\acute{Q}'_\sigma(E)|\psi\}|_{y=0} = \sigma\frac{\sqrt{\mathrm{i}m}}{\hbar}\{x|\check{K}^{1/2}(E)\big(1-\check{T}_\sigma(E)\big)|\psi\} \tag{27}$$

as the continuity of the wavefunctions and their normal derivatives on the CSOS

$$\langle x, 0|\acute{Q}'_\uparrow(E_0)|\uparrow l\} = \langle x, 0|\acute{Q}'_\downarrow(E_0)|\downarrow l\}$$
$$\partial_y\langle x, y|\acute{Q}'_\uparrow(E_0)|\uparrow l\}|_{y=0} = \partial_y\langle x, y|\acute{Q}'_\downarrow(E_0)|\downarrow l\}|_{y=0}$$

which are built up from the pairs of scattering wavefunctions

$$\Psi_n(x, y) = \begin{cases} \langle x, y|\acute{Q}'_\uparrow(E_0)|\uparrow l\} & y > 0 \\ \langle x, y|\acute{Q}'_\downarrow(E_0)|\downarrow l\} & y < 0\,. \end{cases} \tag{28}$$

$d_H(E_0)$, the maximal number of such linearly independent eigenfunctions $\Psi_l(x, y)$ is at least $d_T(E_0) - d_K(E_0)$ since due to completeness of SOS eigenstates $|n\}$ the mapping $\acute{Q}'_\sigma(E_0)$ is injective on the image $\check{K}^2(E_0)\mathcal{L}$. But this number, $d_H(E_0)$, can be larger than $d_T(E_0) - d_K(E_0)$ (but not larger than $d_T(E_0)$) since there may be some states from the null space of $\check{K}^2(E_0)$ for which the limits $E \to E_0$ of (26) and (27) of the upper ($\sigma = \uparrow$) and lower ($\sigma = \downarrow$) part accidentally match. Therefore we have proved an inequality (21).

Analogously, one can show that the $d'_T(E_0)$ basis vectors $\{\downarrow n^*| \in \mathcal{L}', n = 1, \ldots, d'_T(E_0)$ of the left null space

$$\{\downarrow n^*|\big(1 - \check{T}_\downarrow(E_0)\check{T}_\uparrow(E_0)\big) = 0 \tag{29}$$

are mapped onto conjugated basis of eigenfunctions under the propagator $\grave{P}'_\sigma(E_0)$

$$\Psi^*_n(x, y) = \begin{cases} \{\uparrow n^*|\grave{P}'_\uparrow(E_0)|x, y\rangle & y > 0 \\ \{\downarrow n^*|\grave{P}'_\downarrow(E_0)|x, y\rangle & y < 0 \end{cases} \tag{30}$$

where the counterparts $\{\uparrow n^*|$ are again defined as

$$\{\uparrow n^*| = \{\downarrow n^*|\check{T}_\downarrow(E_0)\,. \tag{31}$$

Generally, these conjugated wavefunctions are continuous and differentiable on the CSOS and are thus eigenfunctions of the Hamiltonian $\hat{H}$ if $|\sigma n^*\} \in \check{K}^2(E_0)\mathcal{L}$, otherwise if $|\sigma n^*\} \in \ker\check{K}^2(E_0)$ the continiouity can be accidentally satisfied in the limit $E \to E_0$ if both contributions (upper and lower) coincide. This happens when the corresponding limits for $|\sigma n\}$ (26) and (27) coincide since the two cases only differ by a complex conjugation. So, the dimensions of left and right null space of $1 - \check{T}_\downarrow(E_0)\check{T}_\uparrow(E_0)$ should be the same $d_T(E_0) = d'_T(E_0)$.

The operator $\check{T}'(E) = \check{T}_\downarrow(E)\check{T}_\uparrow(E)$ will be called a *quantum Poincaré mapping* and is the product of the two *quantized Poincaré scattering mappings*. We have proved an extremely efficient quantization condition (as we shall show later), namely, the energies where the quantum Poincaré mapping has fixed points (eigenvalue 1) are either: (i) eigenenergies of the Hamiltonian $\hat{H}$ or (ii) thresholds for opening of new channels E'_n (which are already known as a solution of (3) as a prerequisite of the method).

2.4. SOS decomposition of the resolvent of the Hamiltonian

The kernels of the scattering propagators $\{x|\check{T}_\sigma(E)|x'\}$ will henceforth be called CSOS–CSOS propagators. Then we also define: (i) The linear operator $\acute{Q}_\sigma(E)$ from $\mathcal{L}$ to $\mathcal{H}$ and the linear operator $\grave{P}_\sigma(E)$ from $\mathcal{H}$ to $\mathcal{L}$ with the kernels

$$\langle x, y|\acute{Q}_\sigma(E)|\psi\} = \begin{cases} \langle x, y|\acute{Q}'_\sigma(E)|\psi\} & \sigma y \geqslant 0 \\ 0 & \sigma y < 0 \end{cases} \tag{32}$$

$$\{\psi|\grave{P}_\sigma(E)|x, y\rangle = \begin{cases} \{\psi|\grave{P}'_\sigma(E)|x, y\rangle & \sigma y \geqslant 0 \\ 0 & \sigma y < 0 \end{cases} \tag{33}$$

which are called CSOS–CS and CS–CSOS propagators, respectively, and (ii) a linear operator $\hat{G}_0(E)$ over $\mathcal{H}$ with the kernel

$$\langle x, y|\hat{G}_0(E)|x', y'\rangle = \begin{cases} \langle x, y|\hat{G}_\uparrow(E)|x', y'\rangle & y \geqslant 0,\ y' \geqslant 0 \\ \langle x, y|\hat{G}_\downarrow(E)|x', y'\rangle & y \leqslant 0,\ y' \leqslant 0 \\ 0 & yy' < 0 \end{cases} \tag{34}$$

which is called a CS–CS propagator (without crossing the CSOS in between).

Theorem 2a. The energy-dependent quantum propagator (i.e. the resolvent of the Hamiltonian) $\hat{G}(E) = (E - \hat{H})^{-1}$ can be decomposed in terms of the CS–CS propagator—with no intersection with the CSOS $\mathcal{S}_0$—$\hat{G}_0(E)$, CS–CSOS propagator $\grave{P}_\sigma(E)$, CSOS–CS propagator $\acute{Q}_\sigma(E)$, and CSOS–CSOS propagator $\check{T}_\sigma(E)$

$$\hat{G}(E) = \hat{G}_0(E) + \sum_\sigma \acute{Q}_\sigma(E)(1 - \check{T}_{-\sigma}(E)\check{T}_\sigma(E))^{-1}\grave{P}_{-\sigma}(E)$$
$$+ \sum_\sigma \acute{Q}_\sigma(E)(1 - \check{T}_{-\sigma}(E)\check{T}_\sigma(E))^{-1}\check{T}_{-\sigma}(E)\grave{P}_\sigma(E)\,. \tag{35}$$

Quantities $\langle q|\hat{G}_0(E)|q'\rangle$, $\langle q|\acute{Q}_\sigma(E)|x'\}$, $\{x|\grave{P}_\sigma(E)|q'\rangle$ and $\{x|\check{T}_\sigma(E)|x'\}$ should be interpreted as the probability amplitudes to propagate through the σ-side of CS from point q' in CS/x' on CSOS to point q in CS/x on CSOS at energy E and without crossing CSOS in between. Then this decomposition formula can be understood intuitively by expanding the operator $(1-\check{T}_{-\sigma}(E)\check{T}_\sigma(E))^{-1}$ in a geometric series and then using the basic postulates of quantum mechanics about summation of the probability amplitudes of alternative events (different number of crossings of CSOS) and multiplication of the probability amplitudes of consecutive events (sequential crossings of CSOS) [3], since the system which propagates from point q_i to point q_f in CS along continuous path can cross the CSOS arbitrarily many times. (In fact, the number of crossings is *even* if q_i and q_f lie on the same side of CSOS and *odd* otherwise.) Two versions of the proof of this formula are given in [9, 10] while in this paper the proof will be given for more general cases which include the present one in the following two sections.

2.5. Semiclassical limit

In order to find explicit leading-order semiclassical expressions for the CSOS/CS–CSOS/CS propagators it is convenient to express them first in terms of the scattering Green functions in the hybrid representation (17)–(19)

$$\check{T}_\sigma(E) = \frac{i\hbar^2}{m}\check{K}^{1/2}(E)(\check{G}_\sigma(0,0,E) - \check{G}_{\text{free}}(0,0,E))\check{K}^{1/2}(E)$$

$$\langle \boldsymbol{x}, y|\acute{Q}_\sigma(E) = \frac{\hbar}{\sqrt{-\mathrm{i}m}}\theta(\sigma y)\{\boldsymbol{x}|\check{G}_\sigma(y,0,E)\check{K}^{1/2}(E)$$
$$\grave{P}_\sigma(E)|\boldsymbol{x}, y\rangle = \frac{\hbar}{\sqrt{-\mathrm{i}m}}\theta(\sigma y)\check{K}^{1/2}(E)\check{G}_\sigma(0,y,E)|\boldsymbol{x}\}$$

where the fourth propagator $\check{G}_0(y, y', E)$ is already defined in terms of the scattering resolvents (34) and $\theta(y)$ is the well known Heaviside step function. Then define a linear operator called *half-derivative* with the prescription

$$\partial_y^{1/2}\,\mathrm{e}^{ay} = a^{1/2}\,\mathrm{e}^{ay} \qquad \mathrm{Re}\,a^{1/2} \geqslant 0 \tag{36}$$

which is a sensibly defined positive square root of the differential operator ∂_y. This is a non-local operator which can be expressed explicitly for functions $f(y)$ which increase slower that the square root as y goes towards plus or minus infinity,

$$\partial_y^{1/2}f(y) = \frac{1}{\sqrt{-4\pi}}\int_y^\infty \mathrm{d}y'\frac{f(y')-f(y)}{(y'-y)^{3/2}} \qquad \text{or} \qquad \partial_y^{1/2}f(y) = \frac{1}{\sqrt{4\pi}}\int_{-\infty}^y \mathrm{d}y'\frac{f(y)-f(y')}{(y-y')^{3/2}}$$

respectively. Thus for an operator-valued exponential function, $\partial_y^{1/2}\mathrm{e}^{\mathrm{i}\check{K}y} = \sqrt{\mathrm{i}}\check{K}^{1/2}\mathrm{e}^{\mathrm{i}\check{K}y}$. One may use the Schrödinger equation with proper boundary conditions (which were used to derive (17) and (19)) to see that the scattering Green functions with one coordinate in the waveguide may be written as exponential functions in that coordinate

$$\begin{aligned}\check{G}_\sigma(y, y', E) &= \mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y}\check{G}_\sigma(0, y', E)\\ \check{G}_\sigma(y', y, E) &= \check{G}_\sigma(y', 0, E)\,\mathrm{e}^{-\mathrm{i}\sigma\check{K}(E)y}\end{aligned} \qquad \text{if} \quad \sigma y \leqslant 0,\ \sigma y' > 0\,. \tag{37}$$

Using the forms (16), (37) and the definition of half-derivative one may rewrite the propagators in a more useful form

$$\{\boldsymbol{x}|\check{T}_\sigma(E)|\boldsymbol{x}'\} = -\frac{\hbar^2}{\sigma m}\partial_y^{1/2}\partial_{y'}^{1/2}\langle \boldsymbol{x}, y|\hat{G}_\sigma(E) - \hat{G}_{\mathrm{free}}(E)|\boldsymbol{x}', y'\rangle|_{y=0}^{y'=0} \tag{38}$$

$$\langle \boldsymbol{x}, y|\acute{Q}_\sigma(E)|\boldsymbol{x}'\} = \frac{\mathrm{i}\hbar\theta(\sigma y)}{\sqrt{\sigma m}}\partial_{y'}^{1/2}\langle \boldsymbol{x}, y|\hat{G}_\sigma(E)|\boldsymbol{x}', y'\rangle|_{y'=0} \tag{39}$$

$$\{\boldsymbol{x}'|\grave{P}_\sigma(E)|\boldsymbol{x}, y\rangle = \frac{\mathrm{i}\hbar\theta(\sigma y)}{\sqrt{\sigma m}}\partial_{y'}^{1/2}\langle \boldsymbol{x}', y'|\hat{G}_\sigma(E)|\boldsymbol{x}, y\rangle|_{y'=0}\,. \tag{40}$$

From these formulae one can easily derive semiclassical approximations by using the leading-order semiclassical approximation for the energy-dependent Green function (see e.g. [6, 1])

$$\begin{aligned}\langle \boldsymbol{q}|\hat{G}_\sigma(E)|\boldsymbol{q}'\rangle &\cong \frac{2\pi}{(2\pi\mathrm{i}\hbar)^{(f+1)/2}}\sum_j B_j(\boldsymbol{q}, \boldsymbol{q}', E)\,\mathrm{e}^{\mathrm{i}S_j(\boldsymbol{q},\boldsymbol{q}',E)/\hbar-\mathrm{i}\nu_j\pi/2}\\ B_j(\boldsymbol{q}, \boldsymbol{q}', E) &= \left|\det\begin{pmatrix}\partial_{\boldsymbol{q}}\partial_{\boldsymbol{q}'}S_j & \partial_{\boldsymbol{q}}\partial_E S_j\\ \partial_E\partial_{\boldsymbol{q}'}S_j & \partial_E^2 S_j\end{pmatrix}\right|^{1/2} = m\frac{D_j(\boldsymbol{q}, \boldsymbol{q}', E)}{|p_{yj}p'_{yj}|^{1/2}}\\ D_j(\boldsymbol{q}, \boldsymbol{q}', E) &= |\det\partial_{\boldsymbol{x}}\partial_{\boldsymbol{x}'}S_j(\boldsymbol{q}, \boldsymbol{q}', E)|^{1/2}\end{aligned} \tag{41}$$

where the sum is taken over (*usually finitely many*) classical scattering trajectories labelled by j with classical actions $S_j(\boldsymbol{q}, \boldsymbol{q}', E) = \int_j \mathrm{d}\boldsymbol{q}\cdot\boldsymbol{p}$, and Morse indices ν_j which count the number of conjugated points along the orbit j. $p_{yj} = \partial_y S_j$ and $p'_{yj} = -\partial_{y'}S_j$ are the perpendicular (w.r.t. CSOS) projections of the final and initial momenta. Thus using the definition (36) in the *leading semiclassical order* the half derivatives only cancel the square roots of y-momenta if one expresses the root of the $(f+1) \times (f+1)$ determinant B_j in terms of the root of the $(f-1) \times (f-1)$ determinant D_j,

$$\{x|\check{T}_\sigma(E)|x'\} \cong \frac{1}{(2\pi i\hbar)^{(f-1)/2}} \sum_j{}' D_j(x,0,x',0,E)\,\mathrm{e}^{\mathrm{i}S_j(x,0,x',0,E)/\hbar - \mathrm{i}\nu_j\pi/2} \tag{42}$$

$$\langle x,y|\acute{Q}_\sigma(E)|x'\} \cong \frac{\sqrt{2\pi m}\theta(\sigma y)}{(2\pi i\hbar)^{f/2}} \sum_j \frac{D_j(x,y,x',0,E)}{|p_{yj}|^{1/2}}\,\mathrm{e}^{\mathrm{i}S_j(x,y,x',0,E)/\hbar - \mathrm{i}\nu_j\pi/2} \tag{43}$$

$$\{x'|\grave{P}_\sigma(E)|x,y\rangle \cong \frac{\sqrt{2\pi m}\theta(\sigma y)}{(2\pi i\hbar)^{f/2}} \sum_j \frac{D_j(x',0,x,y,E)}{|p_{yj}|^{1/2}}\,\mathrm{e}^{\mathrm{i}S_j(x',0,x,y,E)/\hbar - \mathrm{i}\nu_j\pi/2}\,. \tag{44}$$

In equation (42) the sum $\sum_j'$ is restricted to only classical orbits which strictly leave CSOS and lie entirely on the σ-side of CS. The 'trivial' classical scattering orbits whose y-coordinates are constantly zero are the only classical orbits of the semiclassical *free* Green function $\hat{G}_{\text{free}}(E)$ and are thus cancelled in expression (38) for the propagator $\check{T}_\sigma(E)$. The sums in (43) and (44) contain only the classical orbits which lie entirely on the σ-side of the CS with one end point on the CSOS and the other end point lying in the σ-side of CS. If there was a classical orbit whose part would lie in the waveguide then its y-coordinate should have an extremum there which, however, is impossible since the classical motion in the waveguide is free in the y-direction. The semiclassical expression for the CS–CS propagator without crossing the CSOS is $\langle x,y|\hat{G}_0(E)|x',y'\rangle$, thus according to definition (34) it looks the same as RHS of (41) where the sum now includes only the classical orbits which *do not cross* CSOS. The leading-order asymptotic results (42)–(44) agree with the semiclassical theory of Bogomolny [1].

The *higher-order semiclassical corrections* to CSOS/CS–CSOS/CS propagators can be obtained in a systematic way by (i) inserting a corrected higher-order semiclassical expression for the scattering Green function (41) in the formulae (38)–(40) and (ii) evaluating the half-derivatives in terms of a power series in $\hbar$. I will now show briefly how both steps can be performed systematically.

(i) *The higher-order corrections to semiclassical energy-dependent Green function* $\langle q|\hat{G}_\sigma(E)|q'\rangle$ can be obtained† by multiplying each term of (41) by a correction factor

$$\langle q|\hat{G}_\sigma(E)|q'\rangle = \frac{2\pi}{(2\pi i\hbar)^{(f+1)/2}} \sum_j B_j\,\mathrm{e}^{\mathrm{i}S_j/\hbar - \mathrm{i}\nu_j\pi/2} \sum_{n=0}^{\infty} \hbar^n f_n^j(q,q',E)\,.$$

The corrections f_n^j can be calculated by inserting the whole expression into the Schrödinger equation. Comparing the terms with equal powers of $\hbar$ and integrating along the orbit yields the explicit recursion formulae for the semiclassical corrections

$$f_0^j(q_j(t),q',E) = 1$$

$$f_n^j(q_j(t),q',E) = \frac{i}{2m}(-)^{n\nu_j(q_j(t),q',E)}\,\mathcal{P}\!\int_0^t \mathrm{d}t'(-)^{n\nu_j(q_j(t'),q',E)}\hat{\Delta}_j f_{n-1}^j(q_j(t'),q',E)$$

$$\hat{\Delta}_j f(q,q',E) = B_j^{-1}(q,q',E)\partial_q^2\left[B_j(q,q',E)f(q,q',E)\right]$$

where $q_j(t)$ denotes the classical orbit j with end points q' and q. One must use the sign factors $(-)^{n\nu_j}$ and the Cauchy principal value of the integral in order to avoid infinite contributions each time one passes a singularity—conjugated point.

† A variant of this approach for a time-dependent quantum propagator (without consideration of conjugated points—short-time limit) has been developed by Roncadelli [13], whereas Gaspard and Alonso [4] used another (path-integral) approach to derive an $\hbar$-expansion of the Gutzwiller trace formula.

(ii) A half derivative of a term like $e^{iS/\hbar}f$, where we shall take $S = S_j$, $f = B_j f_n^j$, may be represented as a power series

$$\partial_y^{1/2} e^{iS/\hbar} f = \frac{1}{\sqrt{\hbar}} e^{iS/\hbar} \sum_{n=0}^{\infty} \hbar^n \hat{C}_n f$$

where $\hat{C}_n$ are some linear operators independent of $\hbar$. Taking it twice, $\partial_y^{1/2}\partial_y^{1/2} = \partial_y$, and comparing the terms with the same power of $\hbar$ one obtains the set of equations which determine the operators $\hat{C}_n$

$$\begin{aligned}
&\hat{C}_0^2 = i\partial_y S \\
&\hat{C}_0\hat{C}_1 + \hat{C}_1\hat{C}_0 = \partial_y \\
&\sum_{m=0}^{n} \hat{C}_m \hat{C}_{n-m} = 0 \qquad n \geqslant 2 .
\end{aligned}$$

It is easy to see that $\hat{C}_n$ is an nth-order differential operator. For example, we give explicit expressions for the first two

$$\hat{C}_0 = (i\partial_y S)^{1/2} \qquad \hat{C}_1 = (i\partial_y S)^{1/2}\left(\frac{i\partial_y^2 S_j}{8(\partial_y S)^2} - \frac{i}{2\partial_y S}\partial_y\right) \tag{45}$$

and the *next-to-leading order semiclassical* expression for the quantum CSOS–CSOS propagator

$$\begin{aligned}
\{x|\check{T}_\sigma(E)|x'\} \cong{}& \frac{1}{(2\pi i\hbar)^{(f-1)/2}} \sum_j^{\prime} D_j\, e^{iS_j/\hbar - i\nu_j\pi/2} \\
&\times\left[1 + \hbar\left(f_1^j + \frac{3i\partial_y^2 S_j}{8p_{yj}^2} + \frac{3i\partial_{y'}^2 S_j}{8p_{yj}^{\prime 2}} - \frac{i\partial_y D_j}{2p_{yj}D_j} + \frac{i\partial_{y'} D_j}{2p'_{yj}D_j}\right)\right]
\end{aligned} \tag{46}$$

where all functions on RHS have arguments $(x, 0, x', 0, E)$.

2.6. Symmetry of the CSOS–CSOS propagator

At a given value of energy E one can split the SOS-Hilbert space on two orthogonal components,

$$\mathcal{L} = \mathcal{L}_o(E) \oplus \mathcal{L}_c(E)$$

the (usually finite-dimensional) subspace of open channels and the (usually infinite-dimensional) subspace of closed channels

$$\begin{aligned}
\mathcal{L}_o(E) &= \left\{|\psi\} \in \mathcal{L},\ \{\psi|\check{K}^2(E)|\psi\} \geqslant 0\right\} \\
\mathcal{L}_c(E) &= \left\{|\psi\} \in \mathcal{L},\ \{\psi|\check{K}^2(E)|\psi\} < 0\right\}
\end{aligned}$$

spanned by $\{|n\}, E_n' \leqslant E\}$, and by $\{|n\}, E_n' > E\}$, respectively.

A very useful piece of information about the CSOS–CSOS propagator which can be written in a block form

$$\check{T}_\sigma(E) = \begin{pmatrix} \check{T}_{oo}(E) & \check{T}_{oc}(E) \\ \check{T}_{co}(E) & \check{T}_{cc}(E) \end{pmatrix}$$

can be obtained by comparing the two expressions for scattering wavefunctions, the conjugated equations (9) and (8). Comparing the values and normal derivatives on CSOS one obtains two equations

$$\sqrt{\mp i}\check{K}^{\mp 1/2}(1 \pm \check{T}_\sigma)|\psi\} = \sqrt{\pm i}\check{K}^{\mp 1/2\dagger}(1 \pm \check{T}_\sigma^\dagger)|\psi^*\} .$$

Noting that $\check{K}^{\pm 1/2}\check{K}^{\mp 1/2\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & \pm\mathrm{i} \end{pmatrix}$ and performing some algebra yields

$$\check{T}_{\mathrm{oo}}\check{T}_{\mathrm{oo}}^{\dagger} = \check{T}_{\mathrm{oo}}^{\dagger}\check{T}_{\mathrm{oo}} = 1 \tag{47}$$

$$\mathrm{i}\check{T}_{\mathrm{oo}}\check{T}_{\mathrm{co}}^{\dagger} = \check{T}_{\mathrm{oc}} \tag{48}$$

$$\mathrm{i}\check{T}_{\mathrm{oc}}^{\dagger}\check{T}_{\mathrm{oo}} = \check{T}_{\mathrm{co}} \tag{49}$$

$$\mathrm{i}\check{T}_{\mathrm{co}}\check{T}_{\mathrm{co}}^{\dagger} = \mathrm{i}\check{T}_{\mathrm{oc}}^{\dagger}\check{T}_{\mathrm{oc}} = \check{T}_{\mathrm{cc}} - \check{T}_{\mathrm{cc}}^{\dagger}\,. \tag{50}$$

This is the so-called *generalized unitarity* [14, 12] of a CSOS–CSOS propagator. Note that the open-open part $\check{T}_{\sigma}^{\mathrm{oo}}(E)$ is indeed a unitary operator (47).

Now we give the representation of the CSOS–CSOS propagator in terms of what is called the *reactance matrix* in scattering theory [8]. This also gives a practical recipe for determining the CSOS–CSOS propagators $\check{T}_{\sigma}(E)$. Let $\Psi_{\sigma n}(x, y, E)$ denote the unique wavefunctions which satisfy the Schrödinger equation (4) with boundary conditions

$$\Psi_{\sigma n}(x, 0, E) = \{x|n\} \qquad \Psi_{\sigma n}(x, \sigma\infty, E) = 0$$

where the second condition should be taken on the boundary of CS if the latter is not infinite. Then one can define the *reactance operators* $\check{R}_{\sigma}(E)$ with matrix elements

$$\{l|\check{R}_{\sigma}(E)|n\} = \frac{\sigma}{k_l^{1/2}(E)k_n^{1/2}(E)} \int_{S} \mathrm{d}x\, \Psi_{\sigma l}^{*}(x, y, E)\partial_y \Psi_{\sigma n}(x, y, E)|_{y=0} \tag{51}$$

and show (using equation (8)) that the CSOS–CSOS propagators can be written as

$$\check{T}_{\sigma}(E) = (1 + \mathrm{i}\check{R}_{\sigma}(E))(1 - \mathrm{i}\check{R}_{\sigma}(E))^{-1}\,. \tag{52}$$

In the case of time-reversal symmetry the wavefunctions $\Psi_{\sigma n}(x, y, E)$ are real and one can use Green's theorem to show that then the reactance matrix is symmetric

$$\{l|\check{R}_{\sigma}(E)|n\} = \{n|\check{R}_{\sigma}(E)|l\} \qquad \text{if} \quad \Psi_{\sigma n}(x, y, E) = \Psi_{\sigma n}^{*}(x, y, E)\,.$$

Using representation (52) this then means that the CSOS–CSOS propagator is also symmetric

$$\{l|\check{T}_{\sigma}(E)|n\} = \{n|\check{T}_{\sigma}(E)|l\} \qquad \text{or} \qquad \{x|\check{T}_{\sigma}(E)|x'\} = \{x'|\check{T}_{\sigma}(E)|x\}\,. \tag{53}$$

2.7. *Practical applications and semi-separable systems*

Let us truncate the basis of $\mathcal{C}$ to include all N_o open channels of $\mathcal{C}_o$ and the first N_c closed channels. The truncated ($N = N_o + N_c$)-dimensional matrices with matrix elements $\{l|\check{T}_{\sigma}(E)|n\}$ and $\{l|\check{R}_{\sigma}(E)|n\}$ will be denoted by $T_{\sigma}(E)$ and $R_{\sigma}(E)$, respectively. In practice one should increase N_c until numerical results converge, which is typically the case [14, 12, 11] for very small values of N_c already, so in the semiclassical limit $N \approx N_o$. The practical SOS-quantization condition then reads

$$\det(1 - T_{\downarrow}(E)T_{\uparrow}(E)) = 0\,. \tag{54}$$

Using equation (52) this condition can be formulated in terms of reactance matrices

$$\det(R_{\uparrow}(E) + R_{\downarrow}(E)) = 0\,. \tag{55}$$

In the case of systems having a time-reversal symmetry (that is if $H'(p_x, x, y) = H'(-p_x, x, y)$) the reactance matrix (51) is a complex-symmetric matrix $R_{\sigma}(E) = R_{\sigma}^{T}(E)$ which is written in terms of a purely real matrix $\tilde{R}_{\sigma}(E)$ via

$$R_{\sigma}(E) = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{-\mathrm{i}} \end{pmatrix} \tilde{R}_{\sigma}(E) \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{-\mathrm{i}} \end{pmatrix}$$

where the diagonal elements are N_o and N_c dimensional sub-matrices. The quantization condition (55) can thus be expressed in terms of *purely real symmetric* matrices $\tilde{R}_\sigma(E) = \tilde{R}_\sigma^T(E) = \tilde{R}_\sigma^*(E)$

$$\det(\tilde{R}_\uparrow(E) + \tilde{R}_\downarrow(E)) = 0\,. \tag{56}$$

Equation (56) is much more efficient for numerical calculation of energy spectra (by seeking its zeros) than the original quantization condition (54) since the former involves real arithmetic [11].

There is a generic (in a sense of dynamics) class of the so-called *semi-separable* systems for which reactance matrices can be calculated straightforwardly and hence the quantization condition (56) can be easily implemented. A semi-separable system should be separable (in (x, y) coordinates) on both sides of CSOS (for $y > 0$ and $y < 0$) but it can be discontinuous on CSOS ($\check{H}'(-0) \neq \check{H}'(+0)$). Thus one has two complete sets of *normalized* SOS eigenmodes, first $|n\}_+$ are eigenstates of $\check{H}'(+0)$, and second $|n\}_-$ are eigenstates of $\check{H}'(-0)$. Since the system is separable on both sides one can explicitly calculate the wavefunctions $\Psi_{\sigma n}(q, E)$ by separation of coordinates

$$\begin{aligned}\Psi_{\uparrow n}(x, y, E) &= \phi_{\uparrow n}(y, E)\{x|n\}_+ \qquad & y > 0\\ \Psi_{\downarrow n}(x, y, E) &= \phi_{\downarrow n}(y, E)\{x|n\}_- \qquad & y < 0\end{aligned}$$

where y-dependent parts should be normalized to give $\phi_{\sigma n}(0, E) = 1$. We have the freedom to cut CS slightly above the discontinuity and choose a privileged set $|n\}_+$ with wavenumbers $k_n(E)$. Then we apply (51) to calculate real reactance matrices

$$\begin{aligned}\tilde{R}_{\uparrow nl}(E) &= |k_n(E)|^{-1}\partial_y\phi_{\uparrow n}(0, E)\delta_{nl}\\ \tilde{R}_{\downarrow nl}(E) &= -|k_n(E)k_l(E)|^{-1/2}\sum_j {}_+\{n|j\}_-\, \partial_y\phi_{\downarrow j}(0, E)\, {}_-\{j|l\}_+\,.\end{aligned}$$

The upper is diagonal while the lower includes transformations by means of real orthogonal matrix with elements ${}_-\{l|n\}_+ = {}_+\{n|l\}_-$ which are typically easily calculated knowing the two sets of SOS-eigenmodes. The author has applied this method for numerical calculation of energy levels in the so-called *semi-separable two-dimensional oscillator* [11] which is a *generic nonlinear autonomous dynamical system with two freedoms*. The method turned out to be capable of yielding accurate consecutive energy levels with sequential numbers of the order of *a few ten millions* at the cost of *few minutes* of Convex C3860 CPU time per level.

3. Abstract formulation of the method

In this section we devize a *general* and *abstract* mathematical framework within which one can prove all versions of simply-connected SOS quantization conditions and SOS decompositions of the resolvents of the corresponding Hamilton operators.

Let $\mathcal{M}$ be an arbitrary normed vector space, which will be referred to as *reduced space*. The vectors from reduced space $\mathcal{M}$—*r-vectors* will be written in bold italic and linear operators over reduced space—*r-operators* will have a mathematical accent ˇ. Then we define an r-operator valued function $\check{L}(y, E)$, where y is a real variable and E is a complex *spectral parameter* (e.g. energy), in order to study the following general homogeneous vector differential equation:

$$\left(\partial_y - \check{L}(y, E)\right)\boldsymbol{f}(y) = 0 \tag{57}$$

over the entire real axis $y \in \mathcal{R}$ (or on some finite interval which contains zero). Normalized r-vector valued functions $\boldsymbol{f}(y)$, $\int \mathrm{d}y\|\boldsymbol{f}(y)\|^2 < \infty$, constitute a normed vector space, denoted by $\mathcal{H}$. The values of the spectral parameter E for which (57) has non-trivial solutions in $\mathcal{H}$ are called *generalized eigenvalues* whereas the corresponding r-vector valued functions are called *generalized eigenfunctions* of (57). It will be shown in the next subsection that this problem is equivalent to the time-independent Schrödinger equation for some special choice of $\check{L}(y, E)$. Equation (57) can be solved generally by means of a Green function $\check{G}(y, y', E)$ which is a unique r-operator valued function which solves the inhomogeneous equation

$$\left(\partial_y - \check{L}(y, E)\right)\check{G}(y, y', E) = \delta(y - y')\check{J}(y, E) \tag{58}$$

with boundary conditions

$$\lim_{y\to\pm\infty} \check{G}(y, y', E) = 0 \tag{59}$$

where $\check{J}(y, E)$ is some non-singular r-operator valued function.

Equation (58) may be written in the form $\hat{L}(E)\hat{G}(E) = 1$ where $\hat{L}(E)$ and $\hat{G}(E)$ are the operators over $\mathcal{H}$ with kernels being r-operator valued distributions $\check{J}^{-1}(y, E)(\delta'(y - y') - \check{L}(y, E)\delta(y - y'))$ and $\check{G}(y, y', E)$, respectively. If left and right inverse of $\hat{L}(E)$ exist and coincide then $\hat{G}(E)\hat{L}(E) = 1$, so the Green function satisfies also the 'conjugated' equation

$$\check{G}(y, y', E)\left(\overleftarrow{\partial_{y'}} - \check{L}'(y', E)\right) = -\delta(y - y')\check{J}(y, E) \tag{60}$$

where

$$\check{L}'(y, E) = -\check{J}^{-1}(y, E)\check{L}(y, E)\check{J}(y, E).$$

We shall construct the Green function $\check{G}(y, y', E)$ by means of the Green functions $\check{G}_\sigma(y, y', E)$ of two *generalized scattering* problems which are defined by cutting the y-axis at $y = 0$ and substituting the upper ($y > 0, \sigma = \uparrow = +$)/lower ($y < 0, \sigma = \downarrow = -$) part of the function $\check{L}(y, E)$ by a constant $\check{L}(E) = \check{L}(0, E)$. Therefore these scattering Green functions satisfy

$$\left(\partial_y - \check{L}(y, E)\right)\check{G}_\sigma(y, y', E) = \delta(y - y')\check{J}(y, E) \qquad \text{if} \quad \sigma y > 0 \tag{61}$$

$$\left(\partial_y - \check{L}(0, E)\right)\check{G}_\sigma(y, y', E) = \delta(y - y')\check{J}(y, E) \qquad \text{if} \quad \sigma y \leqslant 0 \tag{62}$$

with boundary conditions

$$\lim_{y\to\sigma\infty} \check{G}_\sigma(y, y', E) = 0\,. \tag{63}$$

The scattering Green function $\check{G}_\sigma(y, y', E)$ can be written explicitly on the $(-\sigma)$-side ($\sigma y \leqslant 0, \sigma y' \leqslant 0$) in terms of the *abstract scattering operator* $\check{T}_\sigma(E)$

$$\check{G}_\sigma(y, y', E) = \mathrm{i}\exp(\check{L}(E)y)\left(\tfrac{1}{2} - \tfrac{1}{2}\mathrm{i}[y - y']\check{J}(0, E) - \check{T}_\sigma(E)\right)\exp(\check{L}'(E)y') \tag{64}$$

where $[y] = \uparrow = +;\ y > 0,\ [y] = \downarrow = -;\ y < 0$ denotes the *side* or *sign*. Equation (64) can also be considered as a unique definition of the abstract scattering operator, or

$$\check{T}_\sigma(E) = \mathrm{i}\check{G}_\sigma(\pm 0, \mp 0, E) + \tfrac{1}{2} \mp \tfrac{1}{2}\mathrm{i}\check{J}(0, E)\,. \tag{65}$$

Theorem 2b. The Green function of (58) $\check{G}(y, y', E)$ can be decomposed in terms of four r-operator valued functions which can be defined by means of the scattering Green functions

$$\check{G}_0(y, y', E) = \delta_{[y][y']}\check{G}_{[y]}(y, y', E) \tag{66}$$

$$\check{Q}(y, E) = \sqrt{\mathrm{i}}[y]\check{G}_{[y]}(y, 0, E) \tag{67}$$

$$\check{P}(y, E) = \sqrt{\mathrm{i}}[y]\check{G}_{[y]}(0, y, E) \tag{68}$$

$$\check{T}(E) = \check{T}_\uparrow(E) + \check{T}_\downarrow(E) = \mathrm{i}\check{G}_\uparrow(\pm 0, \mp 0, E) + \mathrm{i}\check{G}_\downarrow(\mp 0, \pm 0, E) + 1\,. \tag{69}$$

Namely, the decomposition formula reads

$$\check{G}(y, y', E) = \check{G}_0(y, y', E) + \check{Q}(y, E)(1 - \check{T}(E))^{-1}\check{P}(y', E). \tag{70}$$

Proof. One must show that RHS of (70) is the solution of equations (58) and (59). The first term of the RHS is indeed a solution of a inhomogeneous equation (58) with boundary conditions (59) on both sides but it is generally discontinuous at $y = 0$. The second term of the RHS, or its first factor $\check{Q}(y, E)$, is a solution of the homogeneous equation (57) on both sides but it is again discontinuous at $y = 0$. The sum of the two terms is therefore also the solution of the inhomogeneous equation (58). One is left to prove that the sum is continuous at $y = 0$ and therefore a unique solution of (58). For arbitrary function of y we define the difference operator

$$\Delta_y f(y) = f(y + 0) - f(y - 0). \tag{71}$$

Then the straightforward calculation yields

$$\begin{aligned}\Delta_y \check{G}(0, y', E) &= \Delta_y \check{G}_0(0, y', E) + (\Delta_y \check{Q}(0, E))(1 - \check{T}(E))^{-1}\check{P}(y', E)\\ &= \Delta_y \check{G}_0(0, y', E) - [y']\check{G}_{[y']}(0, y', E) = 0\end{aligned}$$

since

$$\Delta_y \check{Q}(0, E) = \sqrt{i}(1 - \check{T}(E)). \tag{72}$$

Theorem 1b. For any generalized eigenvalue E of (57) the operator $\check{T}(E)$ has a fixed point.

Proof. Any generalized eigenfunction of (57) corresponding to the generalized eigenvalue E can be written in a form

$$f(y) = \check{Q}(y, E)\boldsymbol{a} \tag{73}$$

for some non-zero r-vector $\boldsymbol{a} \in \mathcal{M}$. One can write explicitly, $\boldsymbol{a} = \check{Q}^{-1}(0, E)\boldsymbol{f}(0)$ if $\check{Q}(0, E)$ is invertible, or more generally, $\boldsymbol{a} = [\partial_y^r \check{Q}(y, E)]^{-1}\partial_y^r \boldsymbol{f}(y)|_{y=0}$ if $\partial_y^p \check{Q}(y, E)|_{y=0}$ is singular for all $p = 0, 1 \ldots r - 1$. Equation (73) follows from the definition of the r-operator valued function $\check{Q}(y, E)$ in terms of scattering Green functions on the *non-trivial side*. Since the function $\boldsymbol{f}(y)$ is continuous at $y = 0$, $\Delta_y \boldsymbol{f}(0) = 0$, one sees, using equation (72), that $\boldsymbol{a}$ is a fixed point of the operator $\check{T}(E)$,

$$\check{T}(E)\boldsymbol{a} = \boldsymbol{a}.$$

Note that general decomposition formula (70) is invariant with respect to similarity transformations

$$\begin{aligned}&\check{Q}(y, E) \to \check{Q}(y, E)\check{S}\\ &\check{T}(E) \to \check{S}^{-1}\check{T}(E)\check{S}\\ &\check{P}(y, E) \to \check{S}^{-1}\check{P}(y, E)\end{aligned} \tag{74}$$

and transformations

$$\begin{aligned}&\check{Q}(y, E) \to \check{Q}(y, E)\check{Z}\\ &\check{T}(E) - 1 \to \check{Z}(\check{T}(E) - 1)\check{Z}\\ &\check{P}(y, E) \to \check{Z}\check{P}(y, E)\end{aligned} \tag{75}$$

where $\check{S}$ and $\check{Z}$ are any bijective r-operators.

Note that in this section the symbols denoted by letters G, Q, P, and T have different meaning than in section 2. The propagators from section 2 will appear as elements of block matrices in the following subsection.

3.1. Trivial application

For example, let us first cast our ordinary Schrödinger problem (4) and (2) into the abstract form. Here the reduced space should be $\mathcal{M} = \mathcal{L} \oplus \mathcal{L}$, since the Schrödinger equation is of the second order. One should take

$$\check{L}(y, E) = \begin{pmatrix} 0 & -1 \\ \check{K}^2(y, E) & 0 \end{pmatrix} \qquad \check{J}(y, E) = \begin{pmatrix} 0 & -\check{K}^{-1}(E) \\ \check{K}(E) & 0 \end{pmatrix} \tag{76}$$

in (57) and (58) where $\check{K}^2(y, E) = (2m/\hbar^2)(E - \check{H}'(y))$, $\check{K}(E) = \check{K}(0, E)$. Then, referring to the two components $\mathcal{L}$ of $\mathcal{M}$ with indices 1 and 2, $|\psi(y)\} = f_1(y)$ is a solution of the Schrödinger equation $(\partial_y^2 + \check{K}^2(y, E))|\psi(y)\} = 0$ and $-(2m/\hbar^2)\check{G}_{11}(y, y', E)\check{K}^{-1}(E)$ is its normal Green function (13) in a hybrid representation. Comparing scattering ansätze (18) and (64) and using the similarity transformation (75)

$$\check{S} = \begin{pmatrix} \check{K}^{-1/2}(E) & \check{K}^{-1/2}(E) \\ \mathrm{i}\check{K}^{1/2}(E) & -\mathrm{i}\check{K}^{1/2}(E) \end{pmatrix}$$

one obtains the usual CSOS–CSOS propagators in a compact, block form

$$\check{S}^{-1}\check{T}(E)\check{S} = -\begin{pmatrix} 0 & \check{T}_\uparrow(E) \\ \check{T}_\downarrow(E) & 0 \end{pmatrix}. \tag{77}$$

One can also check that the first 'row' of $(\mathrm{i}\hbar/\sqrt{2m})\check{Q}(y, E)\check{S}$ and the first 'column' of $(\mathrm{i}\hbar/\sqrt{2m})\check{S}^{-1}\check{P}(y, E)\check{K}(E)$ can be written as $(\acute{Q}_\downarrow(E), \acute{Q}_\uparrow(E))$ and $(\grave{P}_\uparrow(E), \grave{P}_\downarrow(E))^T$, respectively. It is now easy to check that the 1, 1 component of the general decomposition formula (70) agrees with the more special case (35).

3.2. Non-trivial applications

There is a straightforward non-trivial generalization of application (76), namely, one can include non-relativistic systems which interact with very general external (gauge) fields and thus have Hamiltonians in our canonical coordinates $(\boldsymbol{x}, y)$ of the form

$$\hat{H} = \frac{1}{2m}(-\mathrm{i}\hbar\partial_y - \hat{A}(y))^2 + \hat{H}'(y) \tag{78}$$

where the only restriction for the self-adjoint operators $\hat{A}(y) = A(-\mathrm{i}\hbar\partial_{\boldsymbol{x}}, \boldsymbol{x}, y)$ and $\hat{H}'(y) = H'(-\mathrm{i}\hbar\partial_{\boldsymbol{x}}, \boldsymbol{x}, y)$ is that they should not depend upon $\check{p}_y$ so they can be restricted to act over the small SOS-Hilbert space $\mathcal{L}$. Again we define the reduced space as $\mathcal{M} = \mathcal{L} \oplus \mathcal{L}$ and the Schrödinger equation (4) with (78) can be written as a first-order system (57) where (76) should be replaced by

$$\check{L}(y, E) = \begin{pmatrix} \mathrm{i}\check{A}(y)/\hbar & -1 \\ \check{K}^2(y, E) & \mathrm{i}\check{A}(y)/\hbar \end{pmatrix} \qquad \check{J}(y, E) = \begin{pmatrix} 0 & -\check{K}^{-1}(E) \\ \check{K}(E) & 0 \end{pmatrix}$$

where all statements from the previous example remain valid except that now the CSOS–CSOS propagator *cannot be separated into upper and lower parts* like (77) and all blocks of $\check{T}(E)$ are generally non-zero.

As for another interesting application one can decompose the Green function of a relativistic Dirac $\frac{1}{2}$-spin fermion bound in an external electromagnetic field $A^\mu(\boldsymbol{x}, y)$ and search for its stationary states. One may choose, for example, $\boldsymbol{x} = (x^1, x^2)$, $y = x^3$ and $\check{L}(y, E) = \gamma^3(\gamma^0(-\mathrm{i}E + \mathrm{i}eA^0) + \gamma^1(\partial_1 - \mathrm{i}eA^1) + \gamma^2(\partial_2 - \mathrm{i}eA^2) + \mathrm{i}m) + \mathrm{i}eA^3$, $\check{J} = -\gamma^3$, so that (57) and (58) reduce to a Dirac equation where $\hbar = c = 1$. The reduced Hilbert space is now the space of Dirac spinor-valued functions over the two-dimensional plane (x^1, x^2).

4. Multiple sections

In this section I consider the case of multiply-connected CSOS. Let CSOS, which is now a smooth multi-sheeted $(f-1)$-dimensional manifold $\mathcal{S}$, divide the f-dimensional CS $\mathcal{C}$ on countably-many disconnected parts whose closures are denoted by $\mathcal{C}_\alpha$, $\alpha \in \mathcal{J}$,

$$\mathcal{C} = \bigcup_{\alpha \in \mathcal{J}} \mathcal{C}_\alpha$$

where $\mathcal{J}$ is some finite or countable index set. Two points are in the same compartment $\mathcal{C}_\alpha$ if they can be connected by a continuous curve which does not cross CSOS $\mathcal{S}$. The compartments $\mathcal{C}_\alpha$ and $\mathcal{C}_\beta$ are said to be neighbouring (denoted by $\alpha|\beta$) if their intersection $\mathcal{S}_{\alpha\beta}$ is a non-empty $(f-1)$-dimensional manifold

$$\alpha|\beta \Leftrightarrow \mathcal{C}_\alpha \cap \mathcal{C}_\beta = \mathcal{S}_{\alpha\beta} \neq \emptyset .$$

The union of all such intersections is the whole CSOS

$$\mathcal{S} = \bigcup_{\alpha|\beta} \mathcal{S}_{\alpha\beta} .$$

$\hat{H}$ is a self-adjoint operator over the Hilbert space $\mathcal{H} = L^2(\mathcal{C})$. Let $\mathcal{O}_{\alpha\beta}, \alpha|\beta$ be open sets which cover the connected parts of CSOS, $\mathcal{S}_{\alpha\beta} \subset \mathcal{O}_{\alpha\beta}$. The Hamiltonian operator $\hat{H}$ is admissible if there exist coordinates $(\boldsymbol{x}, y)_{\alpha\beta}$ for each of the sets $\mathcal{O}_{\alpha\beta}$ such that

$$\begin{aligned} \hat{H}|_{L^2(\mathcal{O}_{\alpha\beta})} &= -\tfrac{1}{2}\hbar^2 \partial_y \hat{M}^{-1}_{\alpha\beta}(y) \partial_y + \hat{H}'_{\alpha\beta}(y) \\ \hat{M}_{\alpha\beta}(y) &= M_{\alpha\beta}(-\mathrm{i}\hbar\partial_{\boldsymbol{x}}, \boldsymbol{x}, y) \\ \hat{H}'_{\alpha\beta}(y) &= H'_{\alpha\beta}(-\mathrm{i}\hbar\partial_{\boldsymbol{x}}, \boldsymbol{x}, y) . \end{aligned} \tag{79}$$

We choose the sign of coordinate y of $\mathcal{O}_{\alpha\beta}$ so that $(\boldsymbol{x}, y)_{\alpha\beta} \in \mathcal{C}_\beta$ if $y > 0$. Here we have allowed for very general 'masses' $\hat{M}_{\alpha\beta}(y)$, which should, of course, be positive operators and hence invertible, which is another generalization of this section. Then I introduce small SOS-Hilbert spaces $\mathcal{L}_{\alpha\beta} = L^2(\mathcal{S}_{\alpha\beta})$, $\alpha|\beta$. The operators restricted to $\mathcal{L}_{\alpha\beta}$ will be again denoted by an accent ˇ. Now cut off the CS around $\mathcal{C}_\alpha$ and attach y-flat the so-called $\alpha\beta$-waveguides on the other sides of all connected parts $\mathcal{S}_{\alpha\beta}$, $\alpha|\beta$ of the boundary $\partial\mathcal{C}_\alpha$ (see figure 2). Thus one defines the scattering Hamiltonians which in local coordinates read

$$\hat{H}_\alpha|_{L^2(\mathcal{O}_{\alpha\beta})} = \begin{cases} -(\hbar^2/2)\partial_y \hat{M}^{-1}_{\alpha\beta}(y)\partial_y + \hat{H}'_{\alpha\beta}(y) & y < 0 \\ -(\hbar^2/2)\partial_y \hat{M}^{-1}_{\alpha\beta}(0)\partial_y + \hat{H}'_{\alpha\beta}(0) & y \geqslant 0 \end{cases} \qquad \alpha|\beta . \tag{80}$$

The fundamental solution of the time-independent Schrödinger equation for the scattering problem (80) in the $\alpha\beta$-waveguide is given by

$${}_{\beta\alpha}\{\boldsymbol{x}|\check{M}^{1/2}_{\alpha\beta}(0)\check{K}^{-1/2}_{\alpha\beta}(E)\, \mathrm{e}^{\pm\mathrm{i}\check{K}_{\alpha\beta}(E)y}$$

where the wavenumber operator $\check{K}_{\alpha\beta}(E)$ is the positive square root of the self-adjoint operator

$$\check{K}^2_{\alpha\beta}(E) = \frac{2}{\hbar^2}\check{M}^{1/2}_{\alpha\beta}(0)(E - \check{H}'_{\alpha\beta}(0))\check{M}^{1/2}_{\alpha\beta}(0) . \tag{81}$$

Vectors from the dual space $\mathcal{L}'_{\alpha\beta}$ are written with reversed indices, e.g. ${}_{\beta\alpha}\{\boldsymbol{x}| \in \mathcal{L}'_{\alpha\beta}$. Thus the general scattering wavefunction of the Hamiltonian $\hat{H}_\alpha$ in the $\alpha\beta$-waveguide $(y > 0)$

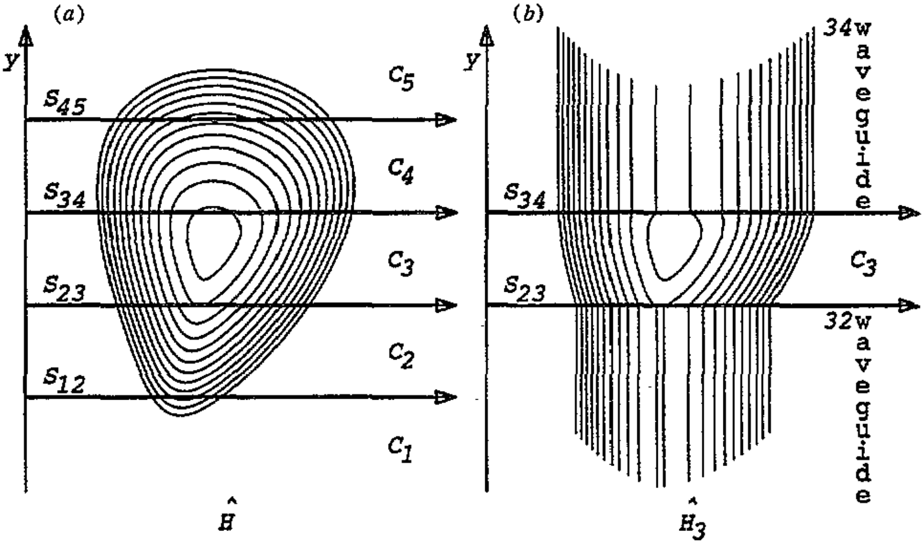

Figure 2. The geometry of the two-dimensional CS of a bound system with multiple sections (a). One of the related scattering systems is shown schematically in (b).

reads

$$\Psi_\alpha(x, y, E) = \frac{\sqrt{-\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{x|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{-1/2}(E)\left[\mathrm{e}^{-\mathrm{i}\check{K}_{\alpha\beta}(E)y}|\psi\}_{\alpha\beta} + \mathrm{e}^{\mathrm{i}\check{K}_{\alpha\beta}(E)y}\sum_{\gamma}^{\gamma|\alpha}\check{T}_{\beta\alpha\gamma}(E)|\psi\}_{\alpha\gamma}\right] \tag{82}$$

$$\Psi_\alpha^*(x, y, E^*) = \frac{\sqrt{-\mathrm{i}}}{\hbar}\left[{}_{\beta\alpha}\{\psi^*|\,\mathrm{e}^{-\mathrm{i}\check{K}_{\alpha\beta}(E)y} + \sum_{\gamma}^{\gamma|\alpha}{}_{\gamma\alpha}\{\psi^*|\check{T}_{\gamma\alpha\beta}(E)\,\mathrm{e}^{\mathrm{i}\check{K}_{\alpha\beta}(E)y}\right] \times\check{K}_{\alpha\beta}^{-1/2}(E)\check{M}_{\alpha\beta}^{1/2}|x\}_{\alpha\beta} \tag{83}$$

(where $\check{M}_{\alpha\beta}^{1/2} = \check{M}_{\alpha\beta}^{1/2}(0)$) and is uniquely determined by the incoming waves parametrized by the SOS-states $|\psi\}_{\alpha\gamma}$ or $|\psi^*\}_{\alpha\gamma}$ coming from the $\alpha\gamma$-waveguide for all neighbouring compartments $\mathcal{C}_\gamma$. We have introduced the scattering operators $\check{T}_{\beta\alpha\gamma}$ which will be called generalized CSOS–CSOS propagators. $\check{T}_{\beta\alpha\gamma}$ is the scattering operator from $\mathcal{L}_{\alpha\gamma}$ to $\mathcal{L}_{\beta\alpha}$ and describes the propagation from $\mathcal{C}_\gamma$ to $\mathcal{C}_\beta$ via $\mathcal{C}_\alpha$. Then we define the two types of linear operators: $\acute{Q}'_{\alpha\gamma}$ from small SOS-Hilbert spaces $\mathcal{L}_{\alpha\gamma}$ to Hilbert space $\mathcal{H}$, and $\grave{P}'_{\gamma\alpha}$ from Hilbert space $\mathcal{H}$ to small SOS-Hilbert spaces $\mathcal{L}_{\gamma\alpha}$ by the following prescriptions:

$$\sum_{\gamma\in\mathcal{J}}^{\gamma|\alpha}\langle q|\acute{Q}'_{\alpha\gamma}(E)|\psi\}_{\alpha\gamma} = \Psi_\alpha(q, E)$$

$$\sum_{\gamma\in\mathcal{J}}^{\gamma|\alpha}{}_{\gamma\alpha}\{\psi^*|\grave{P}'_{\gamma\alpha}(E)|q\rangle = \Psi_\alpha^*(q, E^*)\,.$$

The resolvent of the scattering Hamiltonian with outgoing boundary conditions

$$\hat{G}_\alpha(E) = (E - \hat{H}_\alpha + \mathrm{i}0)^{-1}$$

can also be written explicitly (in analogy with (18)) inside the waveguides ($y \geqslant 0, y' \geqslant 0$)

$$\langle(x, y)_{\alpha\beta}|\hat{G}_\alpha(E)|(x', y')_{\alpha\gamma}\rangle = \frac{1}{i\hbar^2}\ {}_{\beta\alpha}\{x|\check{M}^{1/2}_{\alpha\beta}\check{K}^{-1/2}_{\alpha\beta}(E)\Big[\delta_{\beta\gamma}\, e^{i\check{K}_{\alpha\beta}(E)|y-y'|} + e^{i\check{K}_{\alpha\beta}(E)y}\check{T}_{\beta\alpha\gamma}(E)\, e^{i\check{K}_{\alpha\gamma}(E)y'}\Big]\check{K}^{-1/2}_{\alpha\gamma}(E)\check{M}^{1/2}_{\alpha\gamma}|x'\}_{\alpha\gamma}\,. \tag{84}$$

In analogy with the simply-connected case we also define: (i) the operators $\acute{Q}_{\alpha\gamma}(E)$ from $\mathcal{L}_{\alpha\gamma}$ to $\mathcal{H}$ and the operators $\grave{P}_{\gamma\alpha}(E)$ from $\mathcal{H}$ to $\mathcal{L}_{\gamma\alpha}$ with the kernels

$$\langle q|\acute{Q}_{\alpha\gamma}(E)|\psi\}_{\alpha\gamma} = \begin{cases} \langle q|\acute{Q}'_{\alpha\gamma}(E)|\psi\}_{\alpha\gamma} & q \in \mathcal{C}_\alpha \\ 0 & q \notin \mathcal{C}_\alpha \end{cases} \tag{85}$$

$${}_{\gamma\alpha}\{\psi|\grave{P}_{\gamma\alpha}(E)|q\rangle = \begin{cases} {}_{\gamma\alpha}\{\psi|\grave{P}'_{\gamma\alpha}(E)|q\rangle & q \in \mathcal{C}_\alpha \\ 0 & q \notin \mathcal{C}_\alpha \end{cases} \tag{86}$$

which are called generalized CSOS–CS and CS–CSOS propagators respectively, and (ii) $\hat{G}_0(E)$ a linear operator over $\mathcal{H}$ with the kernel

$$\langle q|\check{G}_0(E)|q'\rangle = \begin{cases} \langle q|\check{G}_\alpha(E)|q'\rangle & \exists\alpha,\ q, q' \in \mathcal{C}_\alpha \\ 0 & \text{otherwise} \end{cases} \tag{87}$$

which is called the generalized CS–CS propagator (without crossing the CSOS in between).

Let us compact our notation by introducing the following symbols. First we define the large SOS-Hilbert space $\mathcal{M}$

$$\mathcal{M} = \bigoplus_{\alpha|\beta} \mathcal{L}_{\alpha\beta}$$

with a complete system of orthogonal projectors $\check{\Pi}_{\alpha\beta}$. (Note that each pair (α, β) is always included twice, once as $\alpha|\beta$ and once as $\beta|\alpha$.) For each SOS-state $|\psi\}$ we write symbolically

$$|\psi\} = \sum_{\alpha|\beta} |\psi\}_{\alpha\beta} \qquad |\psi\}_{\alpha\beta} = \check{\Pi}_{\alpha\beta}|\psi\}\,.$$

One then defines the large operators $\check{T}(E)$, $\acute{Q}(E)$ and $\grave{P}(E)$ by

$$\check{T}(E) = \sum_{\beta|\alpha|\gamma} \check{T}_{\beta\alpha\gamma}(E)\check{\Pi}_{\alpha\gamma}$$

$$\acute{Q}(E) = \sum_{\alpha\gamma} \acute{Q}_{\alpha\gamma}(E)\check{\Pi}_{\alpha\gamma}$$

$$\grave{P}(E) = \sum_{\gamma\alpha} \check{\Pi}_{\gamma\alpha}\grave{P}_{\gamma\alpha}(E)$$

or equivalently

$$\check{\Pi}_{\beta\alpha}\check{T}(E) = \sum_{\gamma\in\mathcal{J}}^{\gamma|\alpha} \check{T}_{\beta\alpha\gamma}(E)\check{\Pi}_{\alpha\gamma} \tag{88}$$

$$\acute{Q}(E)\check{\Pi}_{\alpha\gamma} = \acute{Q}_{\alpha\gamma}(E)\check{\Pi}_{\alpha\gamma} \tag{89}$$

$$\check{\Pi}_{\gamma\alpha}\grave{P}(E) = \check{\Pi}_{\gamma\alpha}\grave{P}_{\gamma\alpha}(E)\,. \tag{90}$$

Now, geometrically most general form of the main result of this paper can be stated and proved very elegantly.

Theorem 2c. The resolvent of the Hamiltonian $\hat{G}(E) = (E - \hat{H})^{-1}$ can be decomposed in terms of four elementary propagators, namely $\hat{G}_0 : \mathcal{H} \to \mathcal{H}$, $\acute{Q} : \mathcal{M} \to \mathcal{H}$, $\grave{Q} : \mathcal{H} \to \mathcal{M}$, and $\check{T} : \mathcal{M} \to \mathcal{M}$, as follows:

$$\hat{G}(E) = \hat{G}_0(E) + \acute{Q}(E)(1 - \check{T}(E))^{-1}\grave{P}(E). \tag{91}$$

Proof. Put the decomposition formula in a sandwitch between $\langle q|$ and $|q'\rangle$. One should prove that the RHS also solves the inhomogeneous Schrödinger equation as the LHS does

$$(E - H(-\mathrm{i}\hbar\partial_q, q))\langle q|\hat{G}(E)|q'\rangle = \delta(q - q'). \tag{92}$$

This is indeed true in every compartment $\mathcal{C}_\alpha$ separately, where $\langle q|\hat{G}_0(E)|q'\rangle$ is a particular solution and $\langle q|\acute{Q}(E)(1 - \check{T}(E))^{-1}\grave{P}(E)|q'\rangle$ is a solution of the homogeneous equation by construction of the operator $\acute{Q}(E)$. What is left to prove is that the RHS is continuously differentiable on borders between compartments, that is on CSOS $\mathcal{S}$. Take arbitrary neighbouring compartments $\mathcal{C}_\alpha$ and $\mathcal{C}_\beta$ and choose coordinates $(\boldsymbol{x}, y)_{\alpha\beta}$ of an open set $\mathcal{O}_{\alpha\beta}$ which includes $\mathcal{S}_{\alpha\beta}$. We shall need the following values and normal derivatives of the CSOS–CS and CS–CSOS propagators on the $\mathcal{S}_{\alpha\beta}$ which can be obtained directly from (82)–(84),

$$\langle(\boldsymbol{x}, 0)_{\alpha\beta}|\acute{Q}_{\alpha\gamma}(E) = \frac{\sqrt{-\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{\boldsymbol{x}|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{-1/2}(E)\big(\check{T}_{\beta\alpha\gamma}(E) + \delta_{\beta\gamma}\big) \tag{93}$$

$$\partial_y\langle(\boldsymbol{x}, 0)_{\alpha\beta}|\acute{Q}_{\alpha\gamma}(E)|_{y=0} = \frac{\sqrt{\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{\boldsymbol{x}|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{1/2}(E)\big(\check{T}_{\beta\alpha\gamma}(E) - \delta_{\beta\gamma}\big) \tag{94}$$

$$\grave{P}_{\gamma\alpha}(E)|(\boldsymbol{x}, 0)_{\alpha\beta}\rangle = \frac{\sqrt{-\mathrm{i}}}{\hbar}\big(\check{T}_{\gamma\alpha\beta}(E) + \delta_{\beta\gamma}\big)\check{K}_{\alpha\beta}^{-1/2}(E)\check{M}_{\alpha\beta}^{1/2}|\boldsymbol{x}\}_{\alpha\beta} \tag{95}$$

$$\partial_y\grave{P}_{\gamma\alpha}(E)|(\boldsymbol{x}, y)_{\alpha\beta}\rangle|_{y=0} = \frac{\sqrt{\mathrm{i}}}{\hbar}\big(\check{T}_{\gamma\alpha\beta}(E) - \delta_{\beta\gamma}\big)\check{K}_{\alpha\beta}^{1/2}(E)\check{M}_{\alpha\beta}^{1/2}|\boldsymbol{x}\}_{\alpha\beta}. \tag{96}$$

First we shall prove that the RHS of (91) is continuous on all $\mathcal{S}_{\alpha\beta}$, $\alpha|\beta$. Using the difference operator (71) we can write (omitting the argument (E) for the sake of brevity)

$$\begin{aligned}
&\Delta_y\langle(\boldsymbol{x}, 0)_{\alpha\beta}|\hat{G}|q'\rangle - \Delta_y\langle(\boldsymbol{x}, 0)_{\alpha\beta}|\hat{G}_0|q'\rangle \\
&\quad = \langle(\boldsymbol{x}, 0)_{\alpha\beta}|\left(\sum_{\gamma\in\mathcal{J}}^{\gamma|\alpha}\acute{Q}_{\alpha\gamma}\check{\Pi}_{\alpha\gamma} - \sum_{\gamma\in\mathcal{J}}^{\gamma|\beta}\acute{Q}_{\beta\gamma}\check{\Pi}_{\beta\gamma}\right)(1 - \check{T})^{-1}\grave{P}|q'\rangle \\
&\quad = \frac{\sqrt{-\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{\boldsymbol{x}|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{-1/2}\left[\sum_{\gamma\in\mathcal{J}}^{\gamma|\alpha}(\check{T}_{\beta\alpha\gamma} + \delta_{\beta\gamma})\check{\Pi}_{\alpha\gamma} - \sum_{\gamma\in\mathcal{J}}^{\gamma|\beta}(\check{T}_{\alpha\beta\gamma} + \delta_{\alpha\gamma})\check{\Pi}_{\beta\gamma}\right] \\
&\qquad \times(1 - \check{T})^{-1}\grave{P}|q'\rangle \\
&\quad = \frac{\sqrt{-\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{\boldsymbol{x}|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{-1/2}\big[\grave{P}_{\alpha\beta} - \grave{P}_{\beta\alpha}\big]|q'\rangle.
\end{aligned}$$

We have applied equations (93), (88) and (90). Analogously, by applying equations (94), (88) and (90) we get (note also that $(\boldsymbol{x}, y)_{\alpha\beta} = (\boldsymbol{x}, -y)_{\beta\alpha}$)

$$\begin{aligned}
&\Delta_y\partial_y\langle(\boldsymbol{x}, y)_{\alpha\beta}|\hat{G}|q'\rangle|_{y=0} - \Delta_y\partial_y\langle(\boldsymbol{x}, y)_{\alpha\beta}|\hat{G}_0|q'\rangle|_{y=0} \\
&\quad = \frac{\sqrt{\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{\boldsymbol{x}|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{1/2}\left[\sum_{\gamma\in\mathcal{J}}^{\gamma|\alpha}(\check{T}_{\beta\alpha\gamma} - \delta_{\beta\gamma})\check{\Pi}_{\alpha\gamma} + \sum_{\gamma\in\mathcal{J}}^{\gamma|\beta}(\check{T}_{\alpha\beta\gamma} - \delta_{\alpha\gamma})\check{\Pi}_{\beta\gamma}\right] \\
&\qquad \times(1 - \check{T})^{-1}\grave{P}|q'\rangle \\
&\quad = \frac{\sqrt{\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{\boldsymbol{x}|\check{M}_{\alpha\beta}^{1/2}\check{K}_{\alpha\beta}^{1/2}\big[\grave{P}_{\alpha\beta} + \grave{P}_{\beta\alpha}\big]|q'\rangle.
\end{aligned}$$

In order to see that $\Delta_y \langle (x,0)_{\alpha\beta}|\hat{G}|q'\rangle = 0$ and $\Delta_y \partial_y \langle (x,y)_{\alpha\beta}|\hat{G}|q'\rangle|_{y=0} = 0$ one has to prove

$$\langle (x,0)_{\alpha\beta}|\hat{G}_\alpha(E)|q'\rangle = \frac{\sqrt{-\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{x|\check{M}^{1/2}_{\alpha\beta}\check{K}^{-1/2}_{\alpha\beta}(E)\grave{P}_{\beta\alpha}(E)|q'\rangle \tag{97}$$

$$\partial_y \langle (x,y)_{\alpha\beta}|\hat{G}_\alpha(E)|q'\rangle|_{y=0} = \frac{\sqrt{\mathrm{i}}}{\hbar}\ {}_{\beta\alpha}\{x|\check{M}^{1/2}_{\alpha\beta}\check{K}^{1/2}_{\alpha\beta}(E)\grave{P}_{\beta\alpha}(E)|q'\rangle \tag{98}$$

considering the definition of $\hat{G}_0(E)$ in terms of $\hat{G}_\alpha(E)$ (equation (87)). But this is easy. Both, LHSs and RHSs of (97) and (98) satisfy the conjugated Schrödinger equation as functions of q'. The initial data, the values and the normal derivatives of the LHSs and RHSs on any initial surface $(x',0)_{\alpha\gamma}$, $\alpha|\gamma$ also match as can be seen by applying $q' = (x',y')_{\alpha\gamma}$ and (84) to LHSs and (95) and (96) to RHSs. The formulae (97) and (98)/(91) then follow from the uniqueness of the initial-value homogeneous (4)/non-homogeneous (92) Schrödinger problem. □

One can formally expand the decomposition formula (91) in a geometric series or *sum over paths*

$$\hat{G}(E) = \hat{G}_0(E) + \sum_{\alpha_1|\alpha_2\ldots|\alpha_n}^{n\geqslant 2} \acute{Q}_{\alpha_n\alpha_{n-1}}(E)\check{T}_{\alpha_n\alpha_{n-1}\alpha_{n-2}}(E)\ldots\check{T}_{\alpha_3\alpha_2\alpha_1}(E)\grave{P}_{\alpha_2\alpha_1}(E) \tag{99}$$

where each term contains probability amplitudes to propagate from compartment C_{α_1} to $C_{\alpha_2}\ldots$ to C_{α_N}. If one chooses many disconnected parts of CSOS $S_{\alpha_k\alpha_{k+1}}$ which are geometrically close then the propagators $\check{T}_{\alpha\beta\gamma}(E)$ would become simple and they could be asymptotically explicitly calculated, so the formula (99) would turn into a kind of path-integral formula for the energy-dependent quantum propagator. Note that so far the expansion (99) only has a formal and heuristic meaning stimulating physical intuition, and probably quite generally gives a divergent series like many other quantum probability amplitude expansions in physics.

5. Discussion and conclusions

This paper presents a theoretical construction of SOS reduction of quantum dynamics in analogy with the SOS reduction of classical dynamics. However, there is an important difference: in classical dynamics, one should carefully choose SOS such that almost every trajectory crosses it, while in quantum dynamics this is not essential. All theorems work even if CSOS lies in a classically forbidden region although the practical usefulness of the method is expected to be worse then, because of the exponential localization and sensitive dependence on boundary conditions. Moreover, the formalism of section 4 can be easily adapted (by taking two different CSOSs as a single multiply-connected CSOS) to show explicitly that the spectra, as determined by our method, do not depend on the choice of the CSOS, since the corresponding quantum Poincaré mappings are related to each other by a kind of similarity transformation.

The Green function—energy-dependent quantum propagator—has been decomposed in terms of propagators which propagate from CS/CSOS to CS/CSOS. This decomposition formula has been generalized in two ways: (i) for Green functions of arbitrary linear differential systems and (ii) for SOS which consists of more than one disconnected part. The combination of these two generalizations is straightforward so it is not given explicitly in this paper. While this general decomposition formula (equation (91) or even (70)) so far has merely theoretical value, it has a very practical consequence, namely, the SOS-quantization condition. The resolvent of the Hamiltonian $(E-\hat{H})^{-1}$ can have a pole, i.e. eigenenergy E_0, only when the operator $1-\check{T}(E_0)$ is singular, i.e. when *the general quantum Poincaré mapping* $\check{T}(E_0)$ has a fixed point $|\psi\} \in \mathcal{M}$, $\check{T}(E_0)|\psi\} = |\psi\}$. For the more special and common case of section 2 we have $\mathcal{M} = \mathcal{L} \oplus \mathcal{L}$, $\check{T} = \begin{pmatrix} 0 & \check{T}_\uparrow \\ \check{T}_\downarrow & 0 \end{pmatrix}$, and $|\psi\} = \begin{pmatrix} |\uparrow\} \\ |\downarrow\} \end{pmatrix}$, where $|\uparrow\}$ is a fixed point of the quantum Poincaré mapping $\check{T}_\downarrow\check{T}_\uparrow$ and at the same time $|\downarrow\}$ is a fixed point of a similar mapping $\check{T}_\uparrow\check{T}_\downarrow$. This quantization condition can be very efficiently numerically implemented [14, 12, 11]. Since the exact quantum Poincaré mapping is usually difficult to calculate explicitly we describe its semiclassical $\hbar$-expansion and give explicitly the leading (Bogomolny's [1]) and next-to-leading order terms.

Recently I have been informed that one of the results of this paper, namely the SOS quantization condition for two-dimensional Hamiltonian systems of the standard type, has also been obtained independently and subsequently by Rouvinez and Smilansky [12]. In a somewhat different notation they use the same scattering trick and their quantization condition is, in fact, identical to one part of theorem 1a while this theorem further explains the spurious levels which are just the threshold energies for opening of the new channels E'_n. They [12] also give a constructive method for obtaining the eigenfunctions which is equivalent to (28) but they do not derive the more general SOS decomposition of the Green function (theorems 2a–c).

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