General Quantum Surface of Section Method

Tomaž Prosen

Center for Applied Mathematics and Theoretical Physics, University of Maribor, Krekova 2, SLO-62000 Maribor, Slovenia

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 $f$-dim configuration space (CS) along $(f-1)-$dim 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.

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\footnote{1\text{e-mail: Tomaz.Prosen@UNI-MB.Si}}
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 \( f \)-dim 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. The question appeared whether there exists a quantum analogue of surface of section (SOS) reduction of classical dynamics which reduces smooth bound and autonomous Hamiltonian dynamics over \( 2f \)-dim phase space to a discrete Poincaré mapping over only \( (2f - 2) \)-dim SOS.

In the case of quantum billiard systems in two dimensions \((f = 2)\) we have the so called boundary integral method which reduces 2-dim Schrödinger equation to 1-dim integral equation. Its kernel can be interpreted as the quantum bounce map which is a special case of Poincaré mapping. Smilansky and coworkers have developed more general scattering approach for quantization of billiards. They construct exact quantum Poincaré mapping for 2-dim 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 dimension of the matrices that they use is typically of the order of square root of the dimension of the original Hamiltonian matrix. On the other hand Bogomolny succeeded to construct approximate semiclassical Poincaré mapping with respect to arbitrary configurational surface of section for 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 prove also theoretically 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 systematically obtained. The symmetries of quantum Poincaré mapping are discussed and it is explained how the SOS quantization condition can be very efficiently used 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 energy-dependent Schrödinger equation of section 2 and more general cases of nonrelativistic 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 conclude.

Some preliminary results of this project have already been reported. Re-
Recently I have been informed that one of the results of this paper, namely the SOS quantization condition for 2-dim Hamiltonian systems of the standard type, has also been obtained independently and subsequently by other authors \[12\].

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 \(f\)-dim configuration space (CS) \(C\). One should also provide a smooth \((f-1)\)-dim submanifold of CS \(C\) which shall be called configurational surface of section (CSOS) \(S_0\) and denoted by \(S_0\). In this section we consider only 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, \(q = (x, y) \in C\) in such a way that the CSOS is given by a simple constraint \(y = 0\), or \(S_0 = (S, 0)\). 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 \(S_0\). This means that every point in \(S_0\) should be uniquely represented by CSOS coordinates \(x \in S\) which may be more general than Euclidean coordinates \(\mathbb{R}^{f-1}\) (e.g. \((f-1)\) dim sphere \(S^{f-1}\)). In this section we shall assume that \(S_0\) is an orientable manifold so that it cuts the CS \(C\) 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 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 next sections we generalize this class to include Hamiltonians having coordinate-dependent mass (which arise in the curvilinear coordinates which must be used in case of non-flat CSOS) and/or terms linear in \(p_y\) (which appear e.g. due to the presence of 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 \(C\) which obey boundary conditions \(\Psi(\partial C) = 0\) \[1\] and have finite \(L^2\) norm \(\int_C dq |\Psi(q)|^2 < \infty\). We shall use the Dirac’s notation. 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

\[\begin{footnotesize}
\text{2} \text{The more general case of } (2f-2)\text{-dim SOS in } 2f\text{-dim phase space which is not perpendicular to CS cannot be treated within the present approach except in the cases where one can change the phase space coordinates by means of an appropriate canonical transformation.}
\end{footnotesize}\]

\[\begin{footnotesize}
\text{3} \text{In case of infinite CS (e.g. Euclidean space } C = \mathbb{R}^f\text{) we assume that points at infinity belong to the boundary } \partial C.
\end{footnotesize}\]
vectors, e.g. position eigenvectors \( |q\rangle = |x, y\rangle \), \( |q\rangle = \int_C dq |q\rangle \langle q| \Psi \rangle = \int_C dq \Psi(q)|q\rangle \) (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 integrable i.e. \( L^2(\mathbb{C}) \)-function). Every ket \( |\Psi\rangle \in \mathcal{H} \) has a corresponding vector from the dual Hilbert space \( \mathcal{H}' \), that is bra \( \langle \Psi| \in \mathcal{H}' \), \( \langle q|\Psi \rangle = \langle q|\Psi \rangle^* \). We shall use mathematical accent \(^\hat{\cdot} \) to denote linear operators over the Hilbert space \( \mathcal{H} \). Operators of SOS coordinates \( \hat{x} \) and \( \hat{p}_x \), defined by

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

can be viewed also 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 \( S_0 \)

\[
\{x|\hat{x}|\psi\} = x\psi(x), \\
\{x|\hat{p}_x|\psi\} = -i\hbar \partial_x \psi(x).
\]

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

\[
\hat{H} = -\frac{\hbar^2}{2m} \partial_y^2 + \hat{H}'(y), \quad \hat{H}'(y) = H'(-i\hbar \partial_x, x, y).
\]

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

\[
\hat{H}'(0)|n\rangle = E'_n|n\rangle,
\]

which are called \textit{SOS-eigenmodes}, provide a useful (countable \( n = 1, 2, \ldots \)) complete and orthogonal basis for \( \mathcal{L} \) since \( \hat{H}'(0) \) 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 \textit{eigenenergies} \( E \) for which the \textit{Schrödinger equation}

\[
\langle x, y|\hat{H}|\Psi_\sigma(E)\rangle = E\Psi_\sigma(x, y, E)
\]

has nontrivial normalizable solutions — \textit{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 multi-channel scattering theory \[8, 15\].

\(^4\text{In case of non-euclidean SOS they should be replaced by the generators of the corresponding Lie algebra.}\)
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

$$
\hat{H}_\sigma = \begin{cases} 
-(h^2/2m)\partial_y^2 + \hat{H}'(y); & \sigma y \geq 0, \\
-(h^2/2m)\partial_y^2 + \hat{H}'(0); & \sigma y < 0.
\end{cases}
$$

(5)

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

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

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 an infinitely many closed channels with imaginary wavenumbers for which $E'_n > E$. 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 vector $|\psi\rangle$ from the SOS-Hilbert space $\mathcal{L}$ (or by vector $|\psi^*\rangle$ from the dual SOS-Hilbert space $\mathcal{L}'$). $|\psi\rangle \in \mathcal{L}$ essentially parametrize the incoming waves

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

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

$$\langle q|\hat{Q}'_\sigma(E)|\psi\rangle = \Psi'_\sigma(q, E),$$

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

(6)

(7)

On the $\sigma$-side of CS ($\sigma y \geq 0$) the scattering wavefunction satisfies ordinary Schrödinger equation (3) whereas in the waveguide ($\sigma y \leq 0$) it is a superposition of incoming and scattered waves

$$\Psi_\sigma(x, y, E) = \frac{\sqrt{-im}}{\hbar} \sum_{n, l} \{x|n\} k_n^{-1/2}(E) \left[ e^{i\sigma k_n(E)y} \delta_{nl} + e^{-i\sigma k_n(E)y} T_{nl} \right] \{l|\psi\} = \frac{\sqrt{-im}}{\hbar} \{x|K^{-1/2}(E) \left[ e^{i\sigma K(E)y} + e^{-i\sigma K(E)y} T_\sigma(E) \right] |\psi\},$$

$$\Psi'_\sigma(x, y, E^*) = \frac{\sqrt{-im}}{\hbar} \{\psi^*| e^{i\sigma K(E)y} + T_\sigma(E) e^{-i\sigma K(E)y} \hat{K}^{-1/2}(E)|x\}.$$
For the sake of compact notation we have introduced the \textit{wavenumber operator}

\[
\hat{K}(E) = \sum_n k_n(E)|n\{n| = \sqrt{\frac{2m}{\hbar^2}}(E - \hat{H}'(0)).
\]  

\(T_{nl}^\sigma(E)\) is the generalized \textit{scattering matrix} since it includes also closed — non-propagating modes and \(\hat{T}_\sigma(E)\) is the corresponding \textit{scattering operator} over \(\mathcal{L}\)

\[
\hat{T}_\sigma(E) = \sum_{n,l} T_{nl}^\sigma|n\{l|.
\]  

Here I have to make three important notes:

- Conjugated energy \(E^*\) is used in argument of complex conjugated wavefunction \((7)\) in order to make all the relevant operators, e.g. \(\hat{P}_\sigma'(E)\), complex analytic functions of \(E\) rather than \(E^*\).
- The SOS-states \(|\psi^*\rangle\) and \(|\psi\rangle\) are generally different.
- The equation \((8)\) is non-trivial and it does not follow from eq. \((8)\) but it is a consequence of the \textit{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 \((3)\) with outgoing boundary conditions

\[
\hat{G}_\sigma(E) = \frac{1}{i\hbar} \int_0^\infty dt e^{i(E - \hat{H}_\sigma)t}/\hbar = (E - \hat{H}_\sigma + i0)^{-1}.
\]  

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

\[
\{x|\hat{G}_\sigma(y, y', E)|x'\} = \langle x, y|\hat{G}_\sigma(E)|x', y'\rangle.
\]  

Inside the waveguide \((\sigma y \leq 0, \sigma y' \leq 0)\) these hybrid Green functions satisfy the following \textit{“free motion”} Schrödinger equations in both arguments

\[
\partial_y^2 \hat{G}_\sigma(y, y', E) + \hat{K}^2(E)\hat{G}_\sigma(y, y', E) = \frac{2m}{\hbar^2}\delta(y - y'),
\]  

\[
\partial_{y'}^2 \hat{G}_\sigma(y, y', E) + \hat{G}_\sigma(y, y', E)\hat{K}^2(E) = \frac{2m}{\hbar^2}\delta(y - y').
\]  

The general solution of this linear system (in the waveguide) is given by the sum of \textit{particular} — “free motion” solution

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

and general solution of the homogeneous system satisfying outgoing boundary conditions

\[
\hat{G}_\sigma(y, y', E) - \hat{G}_{\text{free}}(y, y', E) = \frac{m}{i\hbar^2}\hat{K}^{-1/2}(E)e^{-i\sigma\hat{K}(E)y}Ae^{-i\sigma\hat{K}(E)y'}\hat{K}^{-1/2}(E).
\]
Their sum \( \{x|\hat{G}_\sigma(y,0,E) \} \) satisfies the Schrödinger equation (4) on the \( \sigma \)–side \( (\sigma y \geq 0) \), so comparing it locally, at \( \sigma y = +0 \), with wavefunctions (8) yields

\[
\Psi_\sigma(x,y,E) = \frac{\hbar}{\sqrt{-im}} \{x|\hat{G}_\sigma(y,0,E) \hat{K}^{1/2}(E)|\psi \}, \quad \sigma y \geq 0,
\]

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

\[
\hat{G}_\sigma(y,y',E) = \frac{m}{ih^2} \hat{K}^{-1/2}(E) \left[ e^{i\hat{K}(E)|y-y'|} + e^{-i\sigma\hat{K}(E)y} \hat{T}_\sigma(E) e^{-i\sigma\hat{K}(E)y'} \right] \hat{K}^{-1/2}(E).
\]

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

\[
\Psi^*_\sigma(x,y,E^*) = \frac{\hbar}{\sqrt{-im}} \{\psi^*|\hat{K}^{1/2}(E)\hat{G}_\sigma(0,y,E)|x\}, \quad \sigma y \geq 0,
\]

and equation (9) follows.

### 2.3 SOS energy quantization

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

**Theorem 1a:** Every energy \( E \) for which the operator \( 1 - \hat{T}_\downarrow(E)\hat{T}_\uparrow(E) \) (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 \( 1 - \hat{T}_\downarrow(E)\hat{T}_\uparrow(E) \) are the same

\[
d_T(E) = \dim \ker(1 - \hat{T}_\downarrow(E)\hat{T}_\uparrow(E)) = \dim \ker(1 - \hat{T}_\downarrow(E)\hat{T}_\uparrow(E))^\dagger
\]

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

\[
\max\{d_H(E),d_K(E)\} \leq d_T(E) \leq d_H(E) + d_K(E).
\]

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

\[
(1 - \hat{T}_\downarrow(E_0)\hat{T}_\uparrow(E_0)) |n\} = 0,
\]
Then one may define another set of $d_T(E_0)$ SOS-states $|\downarrow n\rangle \in \mathcal{L}$ by the prescription

$$|\downarrow n\rangle = \tilde{T}_i(E_0) |\uparrow n\rangle,$$  \hspace{1cm} \text{Eq. (23)}

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

$$|\uparrow n\rangle = \tilde{T}_i(E_0) |\downarrow n\rangle.$$  \hspace{1cm} \text{Eq. (24)}

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

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

where $\tilde{K}^2(E)\mathcal{L} = \ker \tilde{K}^2(E)^\perp$ since $\tilde{K}^2(E)$ is self-adjoint. Let the first $m_K$ vectors $|\uparrow m\rangle$, $m = 1, \ldots, m_K$ lie in $\ker \tilde{K}^2(E)$. In order to make sure that scattering wavefunctions (33) have regular limit $E \to E_0$, since $\tilde{K}^{-1/2}(E)$ is becoming singular if $\ker \tilde{K}^2(E_0) \neq \emptyset$, one should demand

$$(1 + \tilde{T}_\sigma(E_0))|\phi\rangle = 0, \quad \langle \phi | (1 + \tilde{T}_\sigma(E_0)) = 0,$$  \hspace{1cm} \text{Eq. (25)}

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

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

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

$$\left(1 + \tilde{T}_i(E_0)\right) |\uparrow l\rangle = \left(1 + \tilde{T}_\mu(E_0)\right) |\downarrow l\rangle,$$

$$\left(1 - \tilde{T}_i(E_0)\right) |\uparrow l\rangle = -\left(1 - \tilde{T}_\mu(E_0)\right) |\downarrow l\rangle,$$

which can be rewritten using the values of the wavefunctions and their normal derivatives on the CSOS (from 33)

$$\langle x,0 | \dot{Q}_\sigma'(E) | \psi \rangle = \frac{\sqrt{-im}}{\hbar} \{ x | \tilde{K}^{-1/2}(E) \left(1 + \tilde{T}_\sigma(E)\right) | \psi \},$$  \hspace{1cm} \text{Eq. (26)}

$$\partial_y \langle x,y | \dot{Q}_\sigma'(E) | \psi \rangle |_{y=0} = \sigma \frac{\sqrt{-im}}{\hbar} \{ x | \tilde{K}^{1/2}(E) \left(1 - \tilde{T}_\sigma(E)\right) | \psi \}$$  \hspace{1cm} \text{Eq. (27)}

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

$$\langle x,0 | \dot{Q}_i'(E_0) | \uparrow l\rangle = \langle x,0 | \dot{Q}_\mu'(E_0) | \downarrow l\rangle$$

$$\partial_y \langle x,y | \dot{Q}_i'(E_0) | \uparrow l\rangle |_{y=0} = \partial_y \langle x,y | \dot{Q}_\mu'(E_0) | \downarrow l\rangle |_{y=0}.$$
which are built up from the pairs of scattering wavefunctions

\[ \Psi_n(x, y) = \begin{cases} 
\langle x, y|\hat{Q}^\dagger_\sigma(E_0)|\uparrow l \rangle; & y > 0, \\
\langle x, y|\hat{Q}_\sigma(E_0)|\downarrow l \rangle; & y < 0,
\end{cases} \quad (28) \]

d_{H}(E_0), the maximal number of such linearly independent eigenfunctions \( \Psi_i(x, y) \) is at least \( d_T(E_0) - d_K(E_0) \) since due to completeness of SOS-eigenstates \( |n\rangle \) the mapping \( \hat{Q}_\sigma(E_0) \) is injective on the image \( \hat{K}^2(E_0)\mathcal{L} \). 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 \( \hat{K}^2(E_0) \) for which the limits (26,27) 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 \( \langle \downarrow n^* \rangle \in \mathcal{L}, n = 1, \ldots, d'_T(E_0) \) of the left null space

\[ \{ \downarrow n^* \langle 1 - \hat{T}_\downarrow(E_0)\hat{T}_\uparrow(E_0) \rangle = 0. \quad (29) \]

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

\[ \Psi_n(x, y) = \begin{cases} 
\{ \uparrow n^*|\hat{P}_\sigma'(E_0)|x, y\rangle; & y > 0, \\
\{ \downarrow n^*|\hat{P}_\sigma'(E_0)|x, y\rangle; & y < 0,
\end{cases} \quad (30) \]

where the counterparts \( \{ \uparrow n^* \} \) are again defined as

\[ \{ \uparrow n^* \} = \{ \downarrow n^*|\hat{T}_\downarrow(E_0) \}. \quad (31) \]

Generally, these conjugated wavefunctions are continuous and differentiable on the CSOS and are thus eigenfunctions of the Hamiltonian \( \hat{H} \) if \( |\sigma n^*\rangle \in \hat{K}^2(E_0)\mathcal{L} \), otherwise if \( |\sigma n^*\rangle \in \ker \hat{K}^2(E_0) \) the continuity 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 \( |\sigma n\rangle \) (26,27) coincide since the two cases differ only by a complex conjugation. So, the dimensions of left and right null space of \( 1 - \hat{T}_\downarrow(E_0)\hat{T}_\uparrow(E_0) \) should be the same \( d_T(E_0) = d'_T(E_0) \).

The operator \( \hat{T}'(E) = \hat{T}_\downarrow(E)\hat{T}_\uparrow(E) \) will be called quantum Poincaré mapping and it 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 \( \{ x|\hat{T}_\sigma(E)|x' \} \) will henceforth be called CSOS-CSOS propagators. Then we define also: (i) The linear operator \( \hat{Q}_\sigma(E) \) from
\( \mathcal{L} \) to \( \mathcal{H} \) and the linear operator \( \hat{P}_\sigma(E) \) from \( \mathcal{H} \) to \( \mathcal{L} \) with the kernels

\[
\langle x, y | \hat{Q}_\sigma(E) | \psi \rangle = \begin{cases} 
\langle x, y | \hat{Q}_\sigma'(E) | \psi \rangle; & \sigma y \geq 0, \\
0; & \sigma y < 0,
\end{cases} \quad (32)
\]

\[
\{ \psi | \hat{P}_\sigma(E) | x, y \} = \begin{cases} 
\{ \psi | \hat{P}_\sigma'(E) | x, y \}; & \sigma y \geq 0, \\
0; & \sigma y < 0.
\end{cases} \quad (33)
\]

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

\[
\langle x, y | \hat{G}_0(E) | x', y' \rangle = \begin{cases} 
\langle x, y | \hat{G}_1(E) | x', y' \rangle; & y \geq 0, y' \geq 0, \\
\langle x, y | \hat{G}_1(E) | x', y' \rangle; & y \leq 0, y' \leq 0, \\
0; & yy' < 0.
\end{cases} \quad (34)
\]

which is called 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 \( S_0 - \hat{G}_0(E) \), CS–CSOS propagator \( \hat{P}_\sigma(E) \), CSOS–CS propagator \( \hat{Q}_\sigma(E) \), and CSOS–CSOS propagator \( \hat{T}_\sigma(E) \)

\[
\hat{G}(E) = \hat{G}_0(E) + \sum_\sigma \hat{Q}_\sigma(E)(1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E))^{-1}\hat{P}_{-\sigma}(E)
\]

\[
+ \sum_\sigma \hat{Q}_\sigma(E)(1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E))^{-1}\hat{T}_{-\sigma}(E)\hat{P}_\sigma(E). \quad (35)
\]

Quantities \( \langle q | \hat{G}_0(E) | q' \rangle, \langle q | \hat{Q}_\sigma(E) | x' \rangle, \{ x | \hat{P}_\sigma(E) | q' \}, \{ x | \hat{T}_\sigma(E) | x' \} \) should be interpreted as the probability amplitudes to propagate through the \( \sigma \)-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 intuitively understood by expanding the operator \( (1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E))^{-1} \) 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) \( \overline{3} \), 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 \( \overline{4} \) and \( \overline{4} \) 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 \([17,18,19]\)

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

\[
\langle x, y|\hat{Q}_\sigma(E) = \frac{\hbar}{\sqrt{-im}} \theta(\sigma y) \{x|\hat{G}_\sigma(y,0,E) \hat{K}^{1/2}(E),
\]

\[
\hat{P}_\sigma(E)|x, y\rangle = \frac{\hbar}{\sqrt{-im}} \theta(\sigma y) \hat{K}^{1/2}(E) \hat{G}_\sigma(0, y, E)|x\rangle,
\]

where the fourth propagator \(\hat{G}_0(y, y', E)\) 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

\[
\partial_y^{1/2} e^{a y} = a^{1/2} e^{a y}, \quad \text{Re} a^{1/2} \geq 0,
\]

which is a sensibly defined positive square root of the differential operator \(\partial_y\). This is nonlocal operator which can be explicitly expressed for functions \(f(y)\) which increase slower that the square root as \(y\) goes towards plus or minus infinity,

\[
\partial_y^{1/2} f(y) = \frac{1}{\sqrt{-4\pi}} \int_{-\infty}^{\infty} dy' \frac{f(y') - f(y)}{(y' - y)^{3/2}}, \quad \text{or} \quad \partial_y^{1/2} f(y) = \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{y} dy' \frac{f(y) - f(y')}{(y' - y)^{3/2}},
\]

respectively. Thus for an operator valued exponential function, \(\partial_y^{1/2} e^{iKy} = \sqrt{iK}^{1/2} e^{iKy}\).

One may use the Schrödinger equation with proper boundary conditions (which were used to derive eqs. \([17,19]\)) to see that the scattering Green functions with one coordinate in the waveguide may be written as exponential functions in that coordinate

\[
\hat{G}_\sigma(y, y', E) = e^{-i\sigma K(E)y} \hat{f}(y', E), \quad \hat{G}_\sigma(y, y, E) = \hat{g}(y', E) e^{-i\sigma K(E)y}, \quad \text{if} \quad \sigma y \leq 0, \quad \sigma y' > 0,
\]

for some operator valued functions \(\hat{f}\) and \(\hat{g}\). Using the forms \([11,37]\) and the definition of half-derivative one may rewrite the propagators in a more useful form

\[
\{x|\hat{T}_\sigma(E)|x'\} = -\frac{\hbar^2}{\sigma m} \partial_y^{1/2} \partial_y^{1/2} \langle x, y|\hat{G}_\sigma(E) - \hat{G}_{\text{free}}(E)|x', y'\rangle|_{y'=0}, \quad \text{or} \label{eq:38}
\]

\[
\langle x, y|\hat{Q}_\sigma(E)|x'\rangle = -\frac{\hbar \theta(\sigma y)}{\sqrt{\sigma m}} \partial_y^{1/2} \langle x, y|\hat{G}_\sigma(E)|x', y'\rangle|_{y'=0}, \label{eq:39}
\]

\[
\{x'|\hat{P}_\sigma(E)|x, y\} = -\frac{\hbar \theta(\sigma y)}{\sqrt{\sigma m}} \partial_y^{1/2} \langle x', y'|\hat{G}_\sigma(E)|x, y\rangle|_{y'=0}.
\]

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. \([3,11]\))

\[
\langle q|\hat{G}_\sigma(E)|q'\rangle \approx \frac{2\pi}{(2\pi\hbar)^{(J+1)/2}} \sum_j B_j(q, q', E) e^{iS_j(q, q', E)/\hbar - iv_j \pi/2}, \label{eq:41}
\]

\[
B_j(q, q', E) = \left| \det \left( \begin{array}{cc} \partial q \partial q' S_j & \partial q \partial E S_j \\ \partial E \partial q S_j & \partial E^2 S_j \end{array} \right) \right|^{1/2} = m \left| D_j(q, q', E) \right|^{1/2},
\]

\[
D_j(q, q', E) = \left| \det \partial q \partial x S_j(q, q', E) \right|^{1/2},
\]

11
where the sum is taken over (usually finitely many) classical scattering trajectories labeled by \( j \) with classical actions \( S_j(q,q',E) = \int q \cdot dq \cdot p \), and Morse indices \( \nu_j \) which count the number of conjugated points along the orbit \( j \). \( p_{y_j} = \partial_{y_j}S_j \) and \( p'_{y_j} = -\partial_{y_j}S_j \) are the perpendicular (w.r.t. CSOS) projections of the final and initial momenta. Thus using the definition \((\ref{eq:1})\) in the leading semiclassical order the half derivatives only cancel the square roots of \( y \)-momenta if one expresses root of \( (f+1) \times (f+1) \) determinant \( B_j \) in terms of root of \( (f-1) \times (f-1) \) determinant \( D_j \),

\[
\{x|\hat{T}_\sigma(E)|x'\} \cong \frac{1}{(2\pi\hbar)^{(j-1)/2}} \sum_j' \sum_i D_j(x,0,x',0,E)e^{iS_j(x,0,x',0,E)/\hbar-i\nu_j\pi/2}, \tag{42}
\]

\[
\langle x,y|\hat{Q}_\sigma(E)|x'\rangle \cong \frac{i\sqrt{2\pi m\theta(\sigma y)}}{(2\pi\hbar)^{j/2}} \sum_j D_j(x,y,x',0,E)\sqrt{|p'_{y_j}|} e^{iS_j(x,y,x',0,E)/\hbar-i\nu_j\pi/2}, \tag{43}
\]

\[
\{x'|\hat{P}_\sigma(E)|x,y\} \cong \frac{i\sqrt{2\pi m\theta(\sigma y)}}{(2\pi\hbar)^{j/2}} \sum_j D_j(x',0,x,y,E)\sqrt{|p'_{y_j}|} e^{iS_j(x',0,x,y,E)/\hbar-i\nu_j\pi/2}. \tag{44}
\]

In \((\ref{eq:2})\) the sum \( \sum_j' \) is restricted only to classical orbits which strictly leave CSOS and lie entirely on the \( \sigma \)-side of CS. The trivial classical scattering orbit whose \( y \)-coordinate is constantly zero is the only classical orbit of the semiclassical free Green function \( \hat{G}_{\text{free}}(E) \) and is thus canceled in the expression \((\ref{eq:18})\) for the propagator \( \hat{T}_\sigma(E) \). The sums in \((\ref{eq:43},\ref{eq:44})\) contain only the classical orbits which lie entirely on the \( \sigma \)-side of the CS with one end point on the CSOS and the other end point lying in the \( \sigma \)-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 \( y \)-direction. The semiclassical expression for the CS-CS propagator without crossing the CSOS \( \langle x,y|\hat{G}_\sigma(E)|x',y'\rangle \) thus according to definition \((\ref{eq:44})\) looks the same as RHS of \((\ref{eq:11})\) where the sum now includes only the classical orbits which do not cross CSOS. The leading order asymptotic results \((\ref{eq:12},\ref{eq:13},\ref{eq:14})\) agree with the semiclassical theory of Bogomolny \([4]\).

The higher order semiclassical corrections to CSOS/CS-CSOS/CS propagators can be obtained in a systematic way by (i) inserting corrected higher order semiclassical expression for the scattering Green function \((\ref{eq:11})\) in the formulae \((\ref{eq:18},\ref{eq:38},\ref{eq:39})\) and (ii) evaluating the half-derivatives in terms of a power series in \( \hbar \). I will show now briefly how both steps can be systematically performed.

\( ^5 \)A variant of this approach for time-dependent quantum propagator (without consideration of conjugated points – short time limit) has been developed by Roncadelli \([3]\), whereas Gaspard and Alonso \([3]\) used another (path integral) approach to derive \( \hbar \)-expansion of Gutzwiller trace formula.
correction factor

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

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

\[
\begin{align*}
  f_0^j(q_j(t), q', E) & = 1, \\
  f_n^j(q_j(t), q', E) & = \frac{i}{2m} (-)^{n\nu_j} (q_j(t), q', E) P \int_0^t dt' (-)^{n\nu_j} (q_j(t'), q', E) \hat{\Delta}_j f_{n-1}^j(q_j(t'), q', E), \\
  \hat{\Delta}_j f(q, q', E) & = B_j^{-1}(q, q', E) \partial^2_q [B_j(q, q', E) f(q, q', E)],
\end{align*}
\]

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.

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

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

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 \( \hat{C}_n \)

\[
\begin{align*}
  \hat{C}_0^2 & = i \partial_y S, \\
  \hat{C}_0 \hat{C}_1 + \hat{C}_1 \hat{C}_0 & = \partial_y, \\
  \sum_{m=0}^n \hat{C}_m \hat{C}_{n-m} & = 0, \quad n \geq 2.
\end{align*}
\]

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

\[ \hat{C}_0 = (i \partial_y S)^{1/2}, \quad \hat{C}_1 = (i \partial_y S)^{1/2} \left( \frac{i \partial^2_y S_j}{8(\partial_y S)^2} - \frac{i}{2 \partial_y S \partial_y} \right) \tag{45} \]

and the \textit{next-to-leading order semiclassical} expression for the quantum CSOS-CSOS propagator

\[
\begin{align*}
  \{ x | T_n(E) | x' \} & \cong \frac{1}{(2\pi i \hbar)^{(j+1)/2}} \sum_j D_j e^{iS_j/h - i\nu_j \pi/2} \sum_{n=0}^\infty \hbar^n f_n^j(q, q', E) \\
  & \times \left[ 1 + \hbar \left( f_l^j + \frac{3i \partial^2_y S_j}{8p^2_{yj}} + \frac{3i \partial^2_{y'} S_j}{8p^2_{yj'}} - \frac{i \partial_y D_j}{2p_{yj} D_j} + \frac{i \partial_{y'} D_j}{2p'_{yj} D_j} \right) \right]\tag{46}
\end{align*}
\]

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 infinitely dimensional) subspace of closed channels

$$
\mathcal{L}_o(E) = \{|\psi\rangle \in \mathcal{L}, \{\psi|\tilde{K}^2(E)|\psi\rangle \geq 0\},
$$

$$
\mathcal{L}_c(E) = \{|\psi\rangle \in \mathcal{L}, \{\psi|\tilde{K}^2(E)|\psi\rangle < 0\}
$$

spanned by $\{|n\rangle, E_n \leq E\}$, and by $\{|n\rangle, E_n > E\}$, respectively.

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

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

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

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

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

$$
\hat{T}_{oo}\hat{T}_\sigma^{\dagger} = \hat{T}_\sigma^{\dagger}\hat{T}_{oo} = 1, \quad (47)
$$

$$
i\hat{T}_{oo}\hat{T}_{co}^{\dagger} = \hat{T}_{oc}, \quad (48)
$$

$$
i\hat{T}_{oc}\hat{T}_{oo}^{\dagger} = \hat{T}_{co}, \quad (49)
$$

$$
i\hat{T}_{co}\hat{T}_{co}^{\dagger} = i\hat{T}_{oc}^{\dagger}\hat{T}_{oc} = \hat{T}_{cc} - \hat{T}_{cc}^{\dagger}. \quad (50)
$$

This is the so called generalized unitarity [14, 12] of a CSOS-CSOS propagator. Note that the open-open part $\hat{T}_{oo}(E)$ is indeed a unitary operator [17].

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

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

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 $\hat{R}_\sigma(E)$ with matrix elements

$$
\langle l|\hat{R}_\sigma(E)|n\rangle = \int_{k_l^{-1/2}(E)k_n^{-1/2}(E)} dx dy \frac{\sigma}{\int_{k_l^{-1/2}(E)k_n^{-1/2}(E)} dx dy} \Psi_{\sigma l}^*(x, y, E)\partial_y \Psi_{\sigma n}(x, y, E)|_{y=0}, \quad (51)
$$

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

$$
\hat{T}_\sigma(E) = (1 + i\hat{R}_\sigma(E))(1 - i\hat{R}_\sigma(E))^{-1}. \quad (52)
$$
In case of time reversal symmetry the wave-functions $\Psi_{\sigma n}(x, y, E)$ are real and one can use Green’s theorem to show that then the reactance matrix is symmetric

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

Using representation (52) this means that then also the CSOS-CSO S propagator is symmetric

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

### 2.7 Practical applications and semi-separable systems

Let us truncate the basis of $L$ to include all $N_o$ open channels of $L_o$ and the first $N_c$ closed channels. The truncated ($N = N_o + N_c$)−dim matrices with matrix elements $\{l|\tilde{T}_{\sigma}(E)|n\}$ and $\{l|\tilde{R}_{\sigma}(E)|n\}$ 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

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

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

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

In 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

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

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

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

The equation (56) is much more efficient for numerical calculation of energy spectra (by seeking its zeros) than original quantization condition (54) since the former involves real arithmetic [14].

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

$$
\Psi_{\uparrow n}(x, y, E) = \phi_{\uparrow n}(y, E)\{x|n\}^+, \quad y > 0,
$$
$$
\Psi_{\downarrow n}(x, y, E) = \phi_{\downarrow n}(y, E)\{x|n\}^-, \quad y < 0,
$$

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

$$
R_{\uparrow nl}(E) = |k_n(E)|^{-1} \partial_y \phi_{\uparrow n}(0, E) \delta_{nl},
$$
$$
R_{\downarrow nl}(E) = -|k_n(E)k_l(E)|^{-1/2} \sum_j +\{n|j\}^- \partial_y \phi_{\downarrow j}(0, E) -\{j:l\}^+.
$$

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 2-dim oscillator [11] which is a generic nonlinear autonomous dynamical system with two freedoms. The method turned out to be capable of yielding consecutive energy levels with sequential number of the order of $10^6$ (million !) at the cost of few minutes of Convex C3860 CPU time per level.

3 Abstract formulation of the method

In this section we devise 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 and linear operators over reduced space $- r$-operators will wear mathematical accent $\check{}$. Then we define $r$-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

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

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

\[
\left( \partial_y - \hat{L}(y, E) \right) \hat{G}(y, y') = \delta(y - y') \hat{J}
\]

with boundary conditions

\[
\lim_{y \to \pm \infty} \hat{G}(y, y', E) = 0. \tag{59}
\]

where \( \hat{J} \) can be an arbitrary nonsingular \( r \)-operator.

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 \( \mathcal{J}^{-1}(\delta'(y-y') - \hat{L}(y, E)\delta(y-y')) \) and \( \hat{G}(y, y', E) \), 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

\[
\hat{G}(y, y') \left( \overline{\partial_y} - \hat{L}'(y', E) \right) = -\delta(y - y') \hat{J}. \tag{60}
\]

where

\[
\hat{L}'(y, E) = -\mathcal{J}^{-1} \hat{L}(y, E) \mathcal{J}.
\]

We shall construct the Green function \( \hat{G}(y, y', E) \) by means of the Green functions \( \hat{G}_\sigma(y, y', E) \) of two \emph{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 function \( \hat{L}(y, E) \) by a constant \( \hat{L}(E) = \hat{L}(0, E) \). Therefore these scattering Green functions satisfy

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

\[
\left( \partial_y - \hat{L}(0, E) \right) \hat{G}_\sigma(y, y') = \delta(y - y') \hat{J}, \quad \text{if} \quad \sigma y \leq 0, \tag{62}
\]

with boundary conditions

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

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

\[
\hat{G}_\sigma(y, y', E) = i \exp(\hat{L}(E)y) \left( \frac{1}{2} - \frac{i}{2} [y - y'] \hat{J} - \hat{T}_\sigma(E) \right) \exp(\hat{L}'(E)y'), \tag{64}
\]

where \([y] = \uparrow = +, y > 0, [y] = \downarrow = -, y < 0 \) denotes the \emph{side} or \emph{sign}. The equation (64) can be considered also as a unique definition of the abstract scattering operator, or

\[
\hat{T}_\sigma(E) = i \hat{G}_\sigma(\pm 0, + 0, E) + \frac{1}{2} \mp \frac{i}{2} \hat{J}. \tag{65}
\]
Theorem 2b: The Green function of the equation \( \mathcal{G}(y, y', E) \) can be decomposed in terms of four \( r \)-operator valued functions which can be defined by means of the scattering Green functions

\[
\begin{align*}
\mathcal{G}_0(y, y', E) &= \delta_{[y][y']} \mathcal{G}_{[y]}(y, y', E), \\
\mathcal{Q}(y, E) &= \sqrt{i}[y] \mathcal{G}_{[y]}(y, 0, E), \\
\mathcal{P}(y, E) &= \sqrt{i}[y] \mathcal{G}_{[y]}(0, y, E), \\
\mathcal{T}(E) &= \mathcal{T}_t(E) + \mathcal{T}_s(E) = i \mathcal{G}_t(\pm 0, \mp 0, E) + i \mathcal{G}_s(\mp 0, \pm 0, E) + 1.
\end{align*}
\]

Namely, the decomposition formula reads

\[
\mathcal{G}(y, y', E) = \mathcal{G}_0(y, y', E) + \mathcal{Q}(y, E) \left( 1 - \mathcal{T}(E) \right)^{-1} \mathcal{P}(y', E).
\]

Proof: One must show that RHS of (70) is the solution of equations (58, 59). The first term of 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 RHS, or its first factor \( \mathcal{Q}(y, E) \), 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 equation (58). For arbitrary function of \( y \) we define the difference operator

\[
\Delta_y f(y) = f(y + 0) - f(y - 0).
\]

Then the straightforward calculation yields

\[
\Delta_y \mathcal{G}(0, y', E) = \Delta_y \mathcal{G}_0(0, y', E) + \left( \Delta_y \mathcal{Q}(0, E) \right) \left( 1 - \mathcal{T}(E) \right)^{-1} \mathcal{P}(y', E) = \\
= \Delta_y \mathcal{G}_0(0, y', E) - [y'] \mathcal{G}_{[y']} (0, y', E) = 0,
\]

since

\[
\Delta_y \mathcal{Q}(0, E) = \sqrt{i}(1 - \mathcal{T}(E)).
\]

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

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

\[
f(y) = \mathcal{Q}(y, E) a
\]

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

$$\tilde{T}(E)a = a.$$ 

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

$$\tilde{Q}(y, E) \rightarrow \tilde{Q}(y, E) \tilde{S},$$
$$\tilde{T}(E) \rightarrow \tilde{S}^{-1} \tilde{T}(E) \tilde{S},$$
$$\tilde{P}(y, E) \rightarrow \tilde{S}^{-1} \tilde{P}(y, E)$$

and transformations

$$\tilde{Q}(y, E) \rightarrow \tilde{Q}(y, E) \tilde{Z}^{-1},$$
$$\tilde{T}(E) - 1 \rightarrow \tilde{Z}(\tilde{T}(E) - 1) \tilde{Z},$$
$$\tilde{P}(y, E) \rightarrow \tilde{Z}^{-1} \tilde{P}(y, E)$$

where $\tilde{S}, \tilde{Z}$ are any bijective r-operators.

### 3.1 Trivial application

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

$$\tilde{L}(y, E) = \begin{pmatrix} 0 & -1 \\ K^2(y, E) & 0 \end{pmatrix}, \quad \tilde{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

in \([37,55]\) where $K^2(y, E) = (2m/\hbar^2)(E - \tilde{H}(y))$, $\tilde{K}(E) = \tilde{K}(0, E)$. Then, referring to the two components $\mathcal{L}$ of $\mathcal{M}$ with indices 1 and 2, $|\psi(y)\rangle = \mathbf{f}_1(y)$ is a solution of the Schrödinger equation $(\partial_y^2 + \tilde{K}^2(y, E))|\psi(y)\rangle = 0$ and $\tilde{G}(y, y', E) = -(2m/\hbar^2)\tilde{G}_{11}(y, y', E)\tilde{K}^{-1}(E)$ is its normal Green function \([33]\) in hybrid representation. Comparing scattering Ansätze \([48]\) and \([44]\) and using the similarity transformation \([44]\)

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

one obtains

$$\tilde{S}^{-1} \tilde{T}(E) \tilde{S} = \begin{pmatrix} 0 & \tilde{T}(E) \\ \tilde{T}^\dagger(E) & 0 \end{pmatrix}. \quad (77)$$

One can also check that the first “row” of $(i\hbar/\sqrt{2m})\tilde{Q}(y, E)\tilde{S}$ and the first “column” of $(i\hbar/\sqrt{2m})\tilde{S}^{-1} \tilde{P}(y, E)\tilde{K}(E)$ can be written as $(\tilde{Q}_\dagger(E), \tilde{Q}_\dagger(E))$ and $(\tilde{P}_\dagger(E), \tilde{P}_\dagger(E))^T$, respectively. It is now easy to check that 1,1 component of the general decomposition formula \((70)\) agrees with the more special case \([33]\).
3.2 Nontrivial applications

There is a straightforward nontrivial generalization of application (76), namely, one can include nonrelativistic systems which interact with very general external (gauge) fields and have thus Hamiltonians in our canonical coordinates \((x, y)\) of the form

\[
\hat{H} = \frac{1}{2m}(-i\hbar \partial_y - \hat{A}(y))^2 + \hat{H}'(y),
\]

(78)

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

\[
\check{L}(y, E) = \begin{pmatrix}
\frac{i\hat{A}(y)}{\hbar} & -1 \\
\frac{i\hat{A}(y)}{\hbar} & 1
\end{pmatrix}, \quad \check{J} = \begin{pmatrix} 0 & -1 \\
1 & 0 \end{pmatrix}
\]

where all statements from the previous example remain valid except that now the CSOS-CSOS propagator cannot be separated to upper and lower part like (77) and all blocks of \(\check{T}(E)\) are generally nonzero.

As for another interesting application one can decompose the Green function of a relativistic Dirac \(\frac{1}{2}\)-spin fermion bound in external electromagnetic field \(A^\mu(x, y)\) and search for its stationary states. One may choose e.g. \(x = (x^1, x^2), y = x^3\) and

\[
\check{L}(y, E) = \gamma^3(\gamma^0(-iE + ieA^0) + \gamma^1(\partial_1 - ieA^1) + \gamma^2(\partial_2 - ieA^2) + im) + ieA^3, \quad \check{J} = -\gamma^3,
\]

so that equations (57,58) reduce to Dirac equation where \(\hbar = c = 1\). The reduced Hilbert space is now the space of Dirac spinor valued functions over 2-dim 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 \((f - 1)\)-dim manifold \(\mathcal{S}\), divide the \(f\)-dim 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 nonempty \((f - 1)\)-dim manifold

\[
\alpha|\beta \iff \mathcal{C}_\alpha \cap \mathcal{C}_\beta = \mathcal{S}_{\alpha\beta} \neq \emptyset.
\]

The union of all such intersections is the whole CSOS

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

\[
\hat{H}|_{L^2(\mathcal{O}_{\alpha\beta})} = -\frac{1}{2}\hbar^2 \partial_y \hat{M}_{\alpha\beta}^{-1}(y) \partial_y + \hat{H}_{\alpha\beta}'(y), \tag{79}
\]

\[
\hat{M}_{\alpha\beta}(y) = M_{\alpha\beta}(-i\hbar \partial_x, x, y),
\]

\[
\hat{H}_{\alpha\beta}'(y) = H_{\alpha\beta}'(-i\hbar \partial_x, x, y).
\]

We choose the sign of coordinate \(y\) of \(\mathcal{O}_{\alpha\beta}\) so that \((x, y)_{\alpha\beta} \in \mathcal{C}_\beta\) 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 accent “. 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

\[
\hat{H}_{\alpha}|_{L^2(\mathcal{O}_{\alpha\beta})} = \begin{cases} 
-(\hbar^2/2)\partial_y \hat{M}^{-1}_{\alpha\beta}(y) \partial_y + \hat{H}_{\alpha\beta}'(y); & y < 0, \\
-(\hbar^2/2)\partial_y \hat{M}^{-1}_{\alpha\beta}(0) \partial_y + \hat{H}_{\alpha\beta}'(0); & y \geq 0,
\end{cases} \tag{80}
\]

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

\[
\beta_\alpha\{x|\hat{M}^{1/2}_{\alpha\beta}(0)\hat{K}^{-1/2}_{\alpha\beta}(E) e^{\pm iK_{\alpha\beta}(E)y}
\]

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

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

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

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

\[
\Psi^*_\alpha(x, y, E^*) = \sqrt{\frac{-i}{\hbar}} \left[ \beta_\alpha\{\psi^*| e^{-iK_{\alpha\beta}(E)y} + \\
+ \sum_\gamma \gamma_\alpha \{\psi^*| \tilde{T}\gamma_{\alpha\beta}(E) e^{iK_{\alpha\beta}(E)y} \hat{K}^{-1/2}_{\alpha\beta}(E) \hat{M}^{1/2}_{\alpha\beta} |x\}_{\alpha\beta}, \tag{83}
\right.
\]

(where \(\hat{M}^{1/2}_{\alpha\beta} = \hat{M}^{1/2}_{\alpha\beta}(0)\)) 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 $C_\gamma$. We have introduced the scattering operators $\hat{T}_{\beta\alpha\gamma}$ which will be called generalized CSOS-CSOS propagators. $\hat{T}_{\beta\alpha\gamma}$ is the scattering operator from $L_{\alpha\gamma}$ to $L_{\beta\alpha}$ and describes the propagation from $C_\gamma$ to $C_\beta$ via $C_\alpha$. Then we define the two types of linear operators: $\hat{Q}'_{\alpha\gamma}(E)$ from small SOS-Hilbert spaces $L_{\alpha\gamma}$ to Hilbert space $H$, and $\hat{P}'_{\gamma\alpha}(E)$ from Hilbert space $H$ to small SOS-Hilbert spaces $L_{\gamma\alpha}$ by the following prescriptions

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

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

The resolvent of the scattering Hamiltonian with outgoing boundary conditions

$$\hat{G}_\alpha(E) = (E - \hat{H}_\alpha + i0)^{-1}$$

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

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

In analogy with the simply connected case we define also: (i) The operators $\hat{Q}_{\alpha\gamma}(E)$ from $L_{\alpha\gamma}$ to $H$ and the operators $\hat{P}_{\gamma\alpha}(E)$ from $H$ to $L_{\gamma\alpha}$ with the kernels

$$\langle q|\hat{Q}_{\alpha\gamma}(E)|\psi\rangle_{\alpha\gamma} = \left\{ \begin{array}{ll} \langle q|\hat{Q}_{\alpha\gamma}'(E)|\psi\rangle_{\alpha\gamma}; & q \in C_\alpha, \\ 0; & q \notin C_\alpha. \end{array} \right.$$  \hspace{1cm} (85)

$$\gamma_{\alpha}\{\psi|\hat{P}_{\gamma\alpha}(E)|q\} = \left\{ \begin{array}{ll} \gamma_{\alpha}\{\psi|\hat{P}_{\gamma\alpha}'(E)|q\}; & q \in C_\alpha, \\ 0; & q \notin C_\alpha. \end{array} \right.$$  \hspace{1cm} (86)

which are called generalized CSOS-CS and CS-CSOS propagators respectively, and

(ii) $\hat{G}_0(E)$ a linear operator over $H$ with the kernel

$$\langle q|\hat{G}_0(E)|q'\rangle = \left\{ \begin{array}{ll} \langle q|\hat{G}_\alpha(E)|q'\rangle; & \exists \alpha, q, q' \in C_\alpha, \\ 0; & \text{otherwise}. \end{array} \right.$$  \hspace{1cm} (87)

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

Let us compactify 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 \( \Pi_{\alpha\beta} \). (Note that each pair \((\alpha, \beta)\) is always included twice, once as \(\alpha|\beta\) and once as \(\beta|\alpha\).) For each SOS-state \(|\psi\rangle\) we write symbolically

\[ |\psi\rangle = \sum_{\alpha|\beta} |\psi\rangle_{\alpha\beta}, \quad |\psi\rangle_{\alpha\beta} = \Pi_{\alpha\beta}|\psi\rangle. \]

One then defines the large operators \( \hat{T}(E) \), \( \hat{Q}(E) \) and \( \hat{P}(E) \) by

\[
\begin{align*}
\hat{T}(E) &= \sum_{\beta|\alpha\gamma} \hat{T}_{\beta\alpha\gamma}(E)\Pi_{\alpha\gamma}, \\
\hat{Q}(E) &= \sum_{\alpha\gamma} \hat{Q}_{\alpha\gamma}(E)\Pi_{\alpha\gamma}, \\
\hat{P}(E) &= \sum_{\gamma\alpha} \Pi_{\gamma\alpha}\hat{P}_{\gamma\alpha}(E),
\end{align*}
\]

or equivalently

\[
\begin{align*}
\Pi_{\beta\alpha}\hat{T}(E) &= \sum_{\gamma\in\mathcal{J}} \hat{T}_{\beta\alpha\gamma}(E)\Pi_{\alpha\gamma}, \\
\hat{Q}(E)\Pi_{\alpha\gamma} &= \hat{Q}_{\alpha\gamma}(E)\Pi_{\alpha\gamma}, \\
\Pi_{\gamma\alpha}\hat{P}(E) &= \Pi_{\gamma\alpha}\hat{P}_{\gamma\alpha}(E).
\end{align*}
\]

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 \( \hat{G}_0 : \mathcal{H} \to \mathcal{H} \), \( \hat{Q} : \mathcal{M} \to \mathcal{H} \), \( \hat{Q} : \mathcal{H} \to \mathcal{M} \), and \( \hat{T} : \mathcal{M} \to \mathcal{M} \), as follows

\[
\hat{G}(E) = \hat{G}_0(E) + \hat{Q}(E) \left(1 - \hat{T}(E)\right)^{-1} \hat{P}(E).
\]

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

\[
(E - H(-i\hbar\partial_q, q))\langle q | \hat{G}(E)| q' \rangle = \delta(q - q').
\]

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 \( \langle q | \hat{Q}(E)(1 - \hat{T}(E))^{-1}\hat{P}(E)| q' \rangle \) is a solution of the homogeneous equation by construction of operator \( \hat{Q}(E) \). What is left to prove is that RHS is continuously differentiable on borders between compartments, that is on CSOS \( S \). Take arbitrary neighbouring compartments \( \mathcal{C}_\alpha \) and \( \mathcal{C}_\beta \) and choose coordinates \((x, y)_{\alpha\beta}\) of an open set \( \mathcal{O}_{\alpha\beta} \) which includes \( S_{\alpha\beta} \). We shall need the following values and normal derivatives of the CSOS-CS and CS-CSOS propagators on the \( S_{\alpha\beta} \) which...
can be obtained directly from \((82, 83, 84)\)

\[
\langle (x, 0)_{\alpha\beta}| \dot{Q}_{\alpha\gamma}(E) \rangle = \frac{\sqrt{-i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2}(E) \left( \tilde{T}_{\beta\alpha\gamma}(E) + \delta_{\beta\gamma} \right), \quad (93)
\]

\[
\partial_y \langle (x, 0)_{\alpha\beta}| \dot{Q}_{\alpha\gamma}(E) \rangle \big|_{y=0} = \frac{\sqrt{-i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2}(E) \left( \tilde{T}_{\beta\alpha\gamma}(E) - \delta_{\beta\gamma} \right), \quad (94)
\]

\[
\dot{P}_{\gamma\alpha}(E) \rangle \langle (x, 0)_{\alpha\beta} \rangle = \frac{\sqrt{-i}}{\hbar} \left( \tilde{T}_{\gamma\alpha\beta}(E) + \delta_{\beta\gamma} \right) \mathcal{K}_{\alpha\beta}^{-1/2}(E) \mathcal{M}_{\alpha\beta}^{1/2} |x\rangle_{\alpha\beta}, \quad (95)
\]

\[
\partial_y \dot{P}_{\gamma\alpha}(E) \rangle \langle (x, y)_{\alpha\beta} \rangle \big|_{y=0} = \frac{\sqrt{-i}}{\hbar} \left( \tilde{T}_{\gamma\alpha\beta}(E) - \delta_{\beta\gamma} \right) \mathcal{K}_{\alpha\beta}^{-1/2}(E) \mathcal{M}_{\alpha\beta}^{1/2} |x\rangle_{\alpha\beta}. \quad (96)
\]

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

\[
\Delta_y \langle (x, 0)_{\alpha\beta}| \hat{G}| q' \rangle - \Delta_y \langle (x, 0)_{\alpha\beta}| \hat{G}_0| q' \rangle =
\]

\[
= \langle (x, 0)_{\alpha\beta} \rangle \left( \frac{\gamma}{\alpha} \sum_{\gamma \in J} \dot{Q}_{\alpha\gamma} \tilde{\Pi}_{\alpha\gamma} - \frac{\gamma}{\beta} \sum_{\gamma \in J} \dot{Q}_{\beta\gamma} \tilde{\Pi}_{\beta\gamma} \right) \left(1 - \tilde{T}\right)^{-1} \hat{P}| q' \rangle =
\]

\[
= \frac{\sqrt{-i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2} \left[ \sum_{\gamma \in J} (\tilde{T}_{\beta\alpha\gamma} + \delta_{\beta\gamma}) \tilde{\Pi}_{\alpha\gamma} - \sum_{\gamma \in J} (\tilde{T}_{\alpha\beta\gamma} + \delta_{\alpha\gamma}) \tilde{\Pi}_{\beta\gamma} \right] \left(1 - \tilde{T}\right)^{-1} \hat{P}| q' \rangle =
\]

\[
= \frac{\sqrt{-i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2} \tilde{\Pi}_{\alpha\beta} - \tilde{P}_{\alpha\beta} | q' \rangle.
\]

We have applied equations \((93, 88, 90)\). And analogously, by applying equations \((84, 88, 89)\) we get (note also that \((x, y)_{\alpha\beta} = (x, -y)_{\beta\alpha}\)

\[
\Delta_y \partial_y \langle (x, y)_{\alpha\beta}| \hat{G}| q' \rangle \big|_{y=0} = \Delta_y \partial_y \langle (x, y)_{\alpha\beta}| \hat{G}_0| q' \rangle \big|_{y=0} =
\]

\[
= \frac{\sqrt{i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2} \left[ \sum_{\gamma \in J} (\tilde{T}_{\beta\alpha\gamma} - \delta_{\beta\gamma}) \tilde{\Pi}_{\alpha\gamma} + \sum_{\gamma \in J} (\tilde{T}_{\alpha\beta\gamma} - \delta_{\alpha\gamma}) \tilde{\Pi}_{\beta\gamma} \right] \left(1 - \tilde{T}\right)^{-1} \hat{P}| q' \rangle =
\]

\[
= \frac{\sqrt{i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2} \tilde{P}_{\beta\alpha} + \hat{P}_{\beta\alpha} | q' \rangle.
\]

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

\[
\langle (x, 0)_{\alpha\beta}| \hat{G}_\alpha(E)| q' \rangle = \frac{\sqrt{-i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2}(E) \hat{P}_{\beta\alpha}(E)| q' \rangle, \quad (97)
\]

\[
\partial_y \langle (x, y)_{\alpha\beta}| \hat{G}_\alpha(E)| q' \rangle \big|_{y=0} = \frac{\sqrt{i}}{\hbar} \beta \{x | \mathcal{M}_{\alpha\beta}^{1/2} \mathcal{K}_{\alpha\beta}^{-1/2}(E) \hat{P}_{\beta\alpha}(E)| q' \rangle, \quad (98)
\]

considering the definition of \(\hat{G}_0(E)\) in terms of \(\hat{G}_\alpha(E)\) \((77)\). But this is easy. Both, LHSs and RHSs of \((77, 88)\) satisfy the conjugated Schrödinger equation as functions of \(q'\). The initial data — the values and the normal derivatives of LHSs and RHSs on any initial surface \((x, y)_{\alpha\gamma}, \alpha|\gamma\) also match as can be seen by applying \(q' = (x, y)_{\alpha\gamma}\).
and (84) to LHSs and (95,96) to RHSs. Formulas (97,98)/(91) then follow from the uniqueness of the initial value homogeneous (4)/non-homogeneous (92) Schrödinger problem. q.e.d.

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

\[
\hat{G}(E) = \hat{G}_0(E) + \sum_{\alpha_1|\alpha_2|...|\alpha_n}^{n \geq 2} \hat{Q}_{\alpha_n\alpha_{n-1}}(E)\hat{T}_{\alpha_n\alpha_{n-1}\alpha_{n-2}}(E)\ldots\hat{T}_{\alpha_3\alpha_2\alpha_1}(E)\hat{P}_{\alpha_2\alpha_1}(E)
\]

where each term contains probability amplitudes to propagate from compartment \(C_{\alpha_1}\) to \(C_{\alpha_2}\ldots\) to \(C_{\alpha_N}\). If one chooses many disconnected parts of CSOS \(S_{\alpha_k\alpha_{k+1}}\) which are geometrically close then the propagators \(\hat{T}_{\alpha_3\gamma}(E)\) would become simple and they could be asymptotically explicitly calculated, so the formula (99) would turn into a kind of path integral formula for energy dependent quantum propagator.

5 Discussion and conclusions

This paper presents 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 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, formalism of section 4 can be easily adapted (by taking two different CSOs 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 (91) or even (70) has so far merely theoretical value, it has a very practical consequence, namely, 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 \(1 - \hat{T}(E_0)\) is singular, i.e. when \(general quantum Poincaré mapping \hat{T}(E_0)\) has a fixed point \(|\psi\rangle \in \mathcal{M}, \hat{T}(E_0)|\psi\rangle = |\psi\rangle\). For the more special and common case of section 2 we have \(\mathcal{M} = \mathcal{L} \oplus \mathcal{L}, \hat{T} = \begin{pmatrix} 0 & T_\uparrow \\ T_\downarrow & 0 \end{pmatrix}\), and \(|\psi\rangle = \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix}\), where \(|\uparrow\rangle\) is a fixed point of quantum Poincaré mapping \(\hat{T}_\uparrow\hat{T}_\downarrow\) and at the same time \(|\downarrow\rangle\) is a fixed point of a similar mapping \(\hat{T}_\uparrow\hat{T}_\downarrow\). 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.

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Figures

Figure 1 The geometry of 2-dim 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,c) is equal to the classical or quantal Poincaré mapping of a bound system (a).

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