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1994 J. Phys. A: Math. Gen. 27 L709

(http://iopscience.iop.org/0305-4470/27/18/011)

J. Phys. A: Math. Gen. 27 (1994) L709–L714. Printed in the UK

LETTER TO THE EDITOR

Exact quantum surface of section method

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Received 6 July 1994

Abstract. This letter presents exact surface of section reduction of quantum mechanics. The main theoretical result is a decomposition of the resolvent of the autonomous bound Hamiltonian $\hat{H}$, $(E-\hat{H})^{-1}$ in terms of the four propagators which propagate from and/or to Hilbert space over the configuration space (CS) to and/or from Hilbert space over the configurational surface of section (CSOS), which has one dimension less than CS. The exact energy quantization condition can be expressed solely in terms of the CSOS–CSOS propagator. All these newly defined energy-dependent (CS/CSOS)–(CS/CSOS) propagators are expressed in terms of the resolvent of the related scattering Hamiltonian.

After the pioneering work of Bogomolny on the semiclassical surface of section propagators [1] there remained a question whether his beautiful approach could be generalized to exact quantum mechanics [4]. Smilansky and co-workers [2, 7] have developed such a principally exact method for quantization of billiards which is closely related to the theory of quantum scattering. In this letter I present the exact quantum surface of section method for quantization of general non-relativistic Hamiltonians of the standard type which is in fact a generalization of the scattering approach for billiards [2, 7]. A more detailed presentation and some further generalizations of the method are given elsewhere [5, 6].

We study Hamiltonian systems with f-freedoms, living in an f-dim configuration space (CS) $\mathcal{C}$, and consider only the case of the so-called configurational surface of section ‡ (CSOS) $\mathcal{S}_0$ which is an $(f-1)$-dim submanifold of CS $\mathcal{C}$. We fix the CS coordinates $q=(x,y)$, $x\in\mathcal{S}$, $y\in\mathcal{I}\subseteq\mathrm{Re}$ in such a way that the CSOS is given by a simple constraint $y=0$, or $\mathcal{S}_0=(\mathcal{S},0)$, where the CSOS coordinates $x\in\mathcal{S}$ may be more general than the usual Euclidian coordinates $\mathcal{S}=\mathrm{Re}^{f-1}$. The CSOS cuts the CS into two pieces which will be referred to as upper and lower and denoted by the value of the index $\sigma=\uparrow,\downarrow$. In arithmetic expressions, the arrows will have the following values, $\uparrow=+1$, $\downarrow=-1$. The theory presented in this letter will apply to quite general classes of bound Hamiltonians whose kinetic energy is quadratic at least perpendicularly to SOS and which is *more general* than the class of standard Hamiltonians $p^2/2m+V(q)$

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

Even more general Hamiltonians including positionally dependent mass and arbitrary gauge fields (e.g. magnetic field) are considered in [6].

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‡ More general cases can be treated by means of such canonical transformations of coordinates which commute with quantization and eliminate the momenta from the surface of section constraint in $2f$-dim phase space.

0305-4470/94/180709+06$19.50

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 $\Psi(\partial C) = 0$ and have finite norm $\int_C \mathrm{d}q\,|\Psi(q)|^2 < \infty$. The Dirac's notation is used. 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 $|q\rangle = |x, y\rangle$, $|\Psi\rangle = \int_C \mathrm{d}q\,|q\rangle\langle q|\Psi\rangle = \int_C \mathrm{d}q\,\Psi(q)|q\rangle$ (in a symbolic sense, since $|q\rangle$ are not proper vectors, but such expansions are still meaningful iff $\Psi(q)$ is square integrable, i.e. L^2-function). Every ket $|\Psi\rangle \in \mathcal{H}$ has a corresponding vector from the dual Hilbert space $\mathcal{H}'$, that is bra $\langle\Psi| \in \mathcal{H}'$, $\langle\Psi|q\rangle = \langle q|\Psi\rangle^*$. Operators $\hat{x}$ and $\hat{p}_x$ can 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 $\mathcal{S}_0$. Vectors in such SOS-Hilbert space, denoted by $\mathcal{L}$, will be written as $|\psi\}$. Eigenvectors of SOS-position operators $\hat{x}$, $\hat{x}|x'\} = x'|x'\}$ provide a useful complete set of basis vectors of $\mathcal{L}$. The quantum Hamiltonian can be written as

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

where the eigenstates of the inside-CSOS Hamiltonian $\hat{H}'(0)$ restricted to the SOS-Hilbert space $\mathcal{L}$, $|n\} \in \mathcal{L}$ called SOS-eigenmodes

$$\hat{H}'(0)|_{\mathcal{L}}|n\} = E'_n|n\} \tag{3}$$

provide a useful (countable $n = 1, 2, \ldots$) complete and orthogonal basis for $\mathcal{L}$ since $\hat{H}'(0)$ is still a self-adjoint operator with discrete spectrum when its domain is restricted to $\mathcal{L}$. By cutting one half of CS off and attaching a semi-infinite separable channel (flat along the y-axis) instead, one defines the two scattering Hamiltonians

$$\hat{H}_\sigma = \begin{cases} -(\hbar^2/2m)\partial_y^2 + \hat{H}'(y) & \sigma y \geqslant 0 \\ -(\hbar^2/2m)\partial_y^2 + \hat{H}'(0) & \sigma y < 0. \end{cases} \tag{4}$$

General scattering wavefunction of the Hamiltonians (4) is also the solution of the original Schrödinger equation $(E - \hat{H})\Psi_\sigma(x, y, E) = 0$ on the σ-side of CS but on the other side of CS (in the channel) it can be explicitly written as a plane wave decomposition in terms of the SOS-eigenmodes

$$\Psi_\sigma(x, y, E) = \langle x, y|\hat{Q}'_\sigma(E)|\psi\}$$

$$(\text{if } \sigma y \leqslant 0:) = \frac{\sqrt{-\mathrm{i}m}}{\hbar}\sum_{n,l}\{x|n\}k_n^{-1/2}(E)[\mathrm{e}^{\mathrm{i}\sigma k_n(E)y}\delta_{nl} + \mathrm{e}^{-\mathrm{i}\sigma k_n(E)y}T^\sigma_{nl}]\{l|\psi\}$$

$$= \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{x|\hat{K}^{-1/2}(E)[\mathrm{e}^{\mathrm{i}\sigma\hat{K}(E)y} + \mathrm{e}^{-\mathrm{i}\sigma\hat{K}(E)y}\hat{T}_\sigma(E)]|\psi\} \tag{5}$$

$$\Psi^*_\sigma(x, y, E^*) = \{\psi|\hat{P}'_\sigma(E)|x, y\rangle$$

$$(\text{if } \sigma y \leqslant 0:) = \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{\psi|[\mathrm{e}^{\mathrm{i}\sigma\hat{K}(E)y} + \hat{T}_\sigma(E)\mathrm{e}^{-\mathrm{i}\sigma\hat{K}(E)y}]\hat{K}^{-1/2}(E)|x\}. \tag{6}$$

We have introduced two linear operators over $\mathcal{L}$ where the discrete spectrum of the first (*waveoperator*)

$$\hat{K}(E) = \sum_n k_n(E)|n\}\{n| = \sqrt{\frac{2m}{\hbar^2}(E - \hat{H}'(0))} \qquad k_n(E) = \sqrt{\frac{2m}{\hbar^2}(E - E'_n)}. \tag{7}$$

consists of the wavenumbers of the perpendicular motion (with respect to CSOS). Typically, there is a finite number of the so-called open SOS-eigenmodes with real wavenumber, $E_n < E$, and infinitely many closed (or *evanescent*) modes with positive imaginary wavenumber, $E_n > E$.

The second newly defined operator over $\mathcal{L}$ is the CSOS–CSOS propagator $\hat{T}_\sigma(E)$ which is just the S-matrix of the corresponding scattering problem (4)

$$\hat{T}_\sigma(E) = \sum_{nl} T^\sigma_{nl}|n\}\{l|. \tag{8}$$

The scattering wavefunction (5) is a unique function of the expansion coefficients $\{l|\psi\}$, or the SOS-state $|\psi\}$, so the linear operator from $\mathcal{L}$ to $\mathcal{H}$, $\hat{Q}'_\sigma(E)$, and linear operator from $\mathcal{H}$ to $\mathcal{L}$, $\hat{P}'_\sigma(E)$, are well defined. Then we define the CSOS–CS/CS–CSOS propagators—linear operator from/to SOS-Hilbert space $\mathcal{L}$ to/from Hilbert space $\mathcal{H}$—by the following prescriptions

$$\langle x, y|\hat{Q}_\sigma(E)|\psi\} = \begin{cases} \langle x, y|\hat{Q}'_\sigma(E)|\psi\} & \sigma y \geqslant 0 \\ 0 & \sigma y < 0 \end{cases} \tag{9}$$

$$\{\psi|\hat{P}_\sigma(E)|x, y\rangle = \begin{cases} \{\psi|\hat{P}'_\sigma(E)|x, y\rangle & \sigma y \geqslant 0 \\ 0 & \sigma y < 0. \end{cases} \tag{10}$$

I will now show the first important result

Theorem 1. The poles of the resolvent $\hat{G}(E) = (E - \hat{H})^{-1}$ (i.e. the eigenenergies of $\hat{H}$) are in one-to-one correspondence with the points E where the operator $1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E)$ is singular. Even more; the dimensions of the null-spaces of $E - \hat{H}$ and of $1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E)$ are the same†.

Every solution of the Schrödinger equation above/below CSOS can be uniquely represented by some $|\psi_\sigma\} \in \mathcal{L}$ in a form $\Psi_\sigma(x, y, E) = \langle x, y|\hat{Q}_\sigma(E)|\psi_\sigma\}$. If E_0 is such a pole, i.e. a d-times degenerate eigenenergy of the Hamiltonian $\hat{H}$, then the corresponding linearly independent eigenfunctions $\Psi_n(x, y), n = 1 \ldots d$ and their normal derivatives $\partial_y \Psi_n(x, y)$ should be continuous on the CSOS $\mathcal{S}_0$. So, there should exist 2D SOS-states $|\sigma n\} \in \mathcal{L}$, $n = 1 \ldots d$, $\sigma = \uparrow, \downarrow$ such that

$$\Psi_n(x, y) = \begin{cases} \langle x, y|\hat{Q}_\uparrow(E_0)|\uparrow n\} & y > 0 \\ \langle x, y|\hat{Q}_\downarrow(E_0)|\downarrow n\} & y < 0 \end{cases} \tag{11}$$

with

$$\begin{aligned} \langle x, 0|\hat{Q}_\uparrow(E_0)|\uparrow n\} &= \langle x, 0|\hat{Q}_\downarrow(E_0)|\downarrow n\} \\ \partial_y \langle x, y|\hat{Q}_\uparrow(E_0)|\uparrow n\}|_{y\searrow 0} &= \partial_y \langle x, y|\hat{Q}_\downarrow(E_0)|\downarrow n\}|_{y\nearrow 0}. \end{aligned} \tag{12}$$

† Due to technical reasons the energy E should not be exactly equal to the threshold for opening of a new mode, i.e. all $k_n(E) \neq 0$ so that $\hat{K}^{-1/2}(E)$ exists.

Continuity relations (12) can be rewritten by using the results

$$\langle x, 0|\hat{Q}_\sigma(E)|\psi\} = \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{x|\hat{K}^{-1/2}(E)(1+\hat{T}_\sigma(E))|\psi\} \tag{13}$$

$$\partial_y\langle x, y|\hat{Q}_\sigma(E)|\psi\}|_{\sigma y\searrow 0} = \sigma\frac{\sqrt{\mathrm{i}m}}{\hbar}\{x|\hat{K}^{1/2}(E)(1-\hat{T}_\sigma(E))|\psi\}$$

(obtained from expansion (5)), and by using the completeness of position SOS-states $|x\}$,

$$(1+\hat{T}_\uparrow(E_0))|\uparrow n\} = (1+\hat{T}_\downarrow(E_0))|\downarrow n\} \tag{15}$$

$$(1-\hat{T}_\uparrow(E_0))|\uparrow n\} = -(1-\hat{T}_\downarrow(E_0))|\downarrow n\}. \tag{16}$$

Adding and subtracting equations (15) and (16) one obtains important relations

$$\hat{T}_\sigma(E_0)|\sigma n\} = |-\sigma n\} \tag{17}$$

which mean that the operator $1-\hat{T}_{-\sigma}(E_0)\hat{T}_\sigma(E_0)$ is singular with $|\sigma n\}$ being the corresponding right null-vectors

$$(1-\hat{T}_{-\sigma}(E_0)\hat{T}_\sigma(E_0))|\sigma n\} = 0. \tag{18}$$

This is an important SOS-quantization condition. Each d SOS-states $|\sigma n\}$, $n = 1\ldots d$ are linearly independent, since $\sum_n c_n|\sigma n\} = 0$ would imply $\sum_n c_n|\Psi_n\rangle = 0$ due to linearity of relation (11). The null-space of $1-\hat{T}_{-\sigma}(E_0)\hat{T}_\sigma(E_0)$ which is spanned by $|\sigma n\}$, $n = 1\ldots n$ is therefore also d-dimensional. The reasoning (11)–(18) is reversible so the converse also holds: The existence of d-dim null space of $1-\hat{T}_{-\sigma}(E_0)\hat{T}_\sigma(E_0)$ also implies the existence of d-dim eigenspace of $\hat{H}$.

One can also derive the complementary SOS-representation of the complex conjugated eigenfunctions $\Psi_n(x, y)$ which are in analogy with (11) provided by propagators $\hat{P}_\sigma(E_0)$. There exists 2D SOS-states $|\sigma n^*\} \in \mathcal{L}$, $n = 1\ldots d$, $\sigma = \uparrow, \downarrow$, such that

$$\Psi_n^*(x, y) = \begin{cases} \{\uparrow n^*|\hat{P}_\uparrow(E_0)|x, y\rangle & y > 0 \\ \{\downarrow n^*|\hat{P}_\downarrow(E_0)|x, y\rangle & y < 0. \end{cases} \tag{19}$$

Requiring continuity of eigenfunctions and their normal derivatives results in a sequence of formulae completely analogous to (12)–(16) ending with

$$\{\sigma n^*|\hat{T}_\sigma(E_0) = \{-\sigma n^*| \tag{20}$$

and the complementary quantization condition

$$\{-\sigma n^*|(1-\hat{T}_{-\sigma}(E_0)\hat{T}_\sigma(E_0)) = 0. \tag{21}$$

The operator $1-\hat{T}_{-\sigma}(E_0)\hat{T}_\sigma(E_0)$ has therefore left and right null-space of the same dimension d.

Let us now consider the resolvents of the scattering Hamiltonians (4) with outgoing boundary conditions $\hat{G}_\sigma(E) = (1/\mathrm{i}\hbar)\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E-\hat{H}_\sigma)t/\hbar} = (E-\hat{H}_\sigma+\mathrm{i}\epsilon)^{-1}$ which can be again explicitly written inside the channel ($\sigma y \leqslant 0$, $\sigma y' \leqslant 0$)

$$\langle x, y|\hat{G}_\sigma(E)|x', y'\rangle = \frac{m}{\mathrm{i}\hbar^2}\{x'|\hat{K}^{-1/2}(E)[\mathrm{e}^{\mathrm{i}\hat{K}(E)|y-y'|} + \mathrm{e}^{-\mathrm{i}\sigma\hat{K}(E)y}\hat{T}_\sigma(E)\mathrm{e}^{-\mathrm{i}\sigma\hat{K}(E)y'}]\hat{K}^{-1/2}(E)|x\} \tag{22}$$

in accordance with equations (5) and (6). The last propagator we define is the CS–CS propagator (without crossing the CSOS in between) $\hat{G}_0(E)$—linear operator over the Hilbert space $\mathcal{H}$ with the kernel

$$\langle \boldsymbol{x}, y|\hat{G}_0(E)|\boldsymbol{x}', y'\rangle = \begin{cases} \langle \boldsymbol{x}, y|\hat{G}_\uparrow(E)|\boldsymbol{x}', y'\rangle & y \geqslant 0,\ y' \geqslant 0 \\ \langle \boldsymbol{x}, y|\hat{G}_\downarrow(E)|\boldsymbol{x}', y'\rangle & y \leqslant 0,\ y' \leqslant 0 \\ 0 & yy' < 0. \end{cases} \tag{23}$$

Theorem 2. Now I can state the second important result. 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 $\hat{P}^\sigma(E)$, CSOS–CS propagator $\hat{Q}^\sigma(E)$, and CSOS–CSOS propagator $\hat{T}^\sigma(E)$

$$\hat{G}(E) = \hat{G}_0(E) + \sum_\sigma \hat{Q}_\sigma(E)(1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E))^{-1}\hat{P}_{-\sigma}(E)$$
$$+ \sum_\sigma \hat{Q}_\sigma(E)(1 - \hat{T}_{-\sigma}(E)\hat{T}_\sigma(E))^{-1}\hat{T}_{-\sigma}(E)\hat{P}_\sigma(E). \tag{24}$$

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) [3], since the system which propagates from point $\boldsymbol{q}_i$ to point $\boldsymbol{q}_f$ in CS along a continuous path can cross the CSOS arbitrarily many times. (In fact, the number of crossings is *even* if $\boldsymbol{q}_i$ and $\boldsymbol{q}_f$ lie on the same side of CSOS and *odd* otherwise.) The decomposition of the resolvent (24) can be proved by considering two facts: (i) The RHS is also a solution of the Schrödinger equation $(E - \hat{H})\langle \boldsymbol{x}, y|\hat{G}(E)|\boldsymbol{x}'y'\rangle = \delta(\boldsymbol{x} - \boldsymbol{x}')\delta(y - y')$. This is indeed true. The first term of the RHS $\langle \boldsymbol{x}, y|\hat{G}_0(E)|\boldsymbol{x}'y'\rangle$ is the particular solution of the non-homogeneous Schrödinger equation while the remaining terms are solutions of the homogeneous Schrödinger equation apart from discontinuities at $y = 0$. (ii) The RHS is also continuously differentiable at $y = 0$. Using (24), (13) and (14) one can show that this is true if

$$\langle \boldsymbol{x}, 0|\hat{G}_0(E)|\boldsymbol{x}', y'\rangle = \frac{\sqrt{-\mathrm{i}m}}{\hbar}\{\boldsymbol{x}'|\hat{K}^{-1/2}(E)\hat{P}_\sigma(E)|\boldsymbol{x}', y'\rangle \tag{25}$$

$$\partial_y\langle \boldsymbol{x}, y|\hat{G}_0(E)|\boldsymbol{x}', y'\rangle|_{y=0} = -\sigma\frac{\sqrt{\mathrm{i}m}}{\hbar}\{\boldsymbol{x}'|\hat{K}^{1/2}(E)\hat{P}_\sigma(E)|\boldsymbol{x}', y'\rangle \tag{26}$$

where $\sigma = \operatorname{sgn} y'$. The validity of these identities can be checked by verifying: (i) that both LHSs and RHSs satisfy the conjugated Schrödinger equation (as functions of $(\boldsymbol{x}', y')$ and (ii) that their values and their normal derivatives match on the 'initial surface' $\mathcal{S}_0$ (put $y' = 0$) that can be seen by applying (23) and (22) to the LHSs and applying (10) and (6) to the RHSs.

Before we conclude we shall use the relations such as equation (22), equation (25) and its analogue for the propagator $\hat{Q}_\sigma(E)$, and the completeness of the SOS-position states to express the remaining three propagators solely in terms of the scattering resolvent (the fourth propagator $\hat{G}_0(E)$ is already defined in terms of the scattering resolvent (23))

$$\langle \boldsymbol{x}, y|\hat{Q}_\sigma(E) = \frac{\hbar}{\sqrt{-\mathrm{i}m}}\theta(\sigma y)\int_S \mathrm{d}\boldsymbol{x}'\,\langle \boldsymbol{x}, y|\hat{G}_\sigma(E)|\boldsymbol{x}', 0\rangle\{\boldsymbol{x}'|\hat{K}^{1/2}(E) \tag{27}$$

$$\hat{P}_\sigma(E)|x, y\rangle = \frac{\hbar}{\sqrt{-\mathrm{i}m}}\theta(\sigma y)\int_S \mathrm{d}x'\,\hat{K}^{1/2}(E)|x'\}\langle x', 0|\hat{G}_\sigma(E)|x, y\rangle \tag{28}$$

$$\hat{T}_\sigma(E) + 1 = \frac{\mathrm{i}\hbar^2}{m}\int_S\int_S \mathrm{d}x'\,\mathrm{d}x''\,\hat{K}^{1/2}(E)|x'\}\langle x', 0|\hat{G}_\sigma(E)|x'', 0\rangle\{x''|\hat{K}^{1/2}(E) \tag{29}$$

where $\theta(y)$ is a step function, $\theta(y \geqslant 0) = 1$, $\theta(y < 0) = 0$. The representation (29) can be used to obtain the semiclassical limit $\hbar \to 0$ of the CSOS–CSOS propagator by considering the resolvent of the scattering Hamiltonian represented by the Feynman path integral [3] which can be evaluated together with the remaining integrals in (29) by the method of stationary phase giving exactly the Bogomolny's semiclassical SOS propagator [1] in terms of classical orbits (see also [6]).

In this letter I have outlined the exact quantum surface of section method for a large class of Hamiltonians including the standard ones. Even more general treatment is given in [6]. In another paper [5] I have used a different approach to prove the decomposition of the resolvent (24) which is considerably more complicated than the present one but it gives several useful results which cannot be obtained by the direct approach used in this letter. The quantum surface of section method is expected to be numerically very effective [7] if one uses finite truncated basis for $\mathcal{L}$ consisting of all the open modes and the first few closed modes. The problem is how to calculate the CSOS–CSOS propagator $\hat{T}_\sigma(E)$ numerically. It is an easy task only if the problem is separable (although in a different way) on both sides of CSOS. One general idea is to consider a family of surfaces of section $y = y_0$ and the first-order Riccati differential equation for the propagator $\hat{T}_\sigma(E, y_0)$ as a function of y_0 [5].

I am grateful to Professor Marko Robnik for fruitful discussions. The financial support by the Ministry of Science and Technology of the Republic of Slovenia is gratefully acknowledged.

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