Reconstruction of dynamics from an eigenstate

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For Hamiltonians that have a formal (canonical) decomposition $H = -\frac{1}{2}\Delta + V(x)$, $V(x)$ being a multiplication operator, the definition of the dynamics by a ground state measure leads to an energy (Dirichlet) form formulation of quantum mechanics that is more general than the operator Schrödinger approach. Here, the question of reconstruction of the dynamics from an eigenstate when the potential is not restricted to the class of multiplication operators is analyzed. By explicit analysis of several examples, it is found that, once a particular operator class is chosen, the potential and the energy form are, to some extent, determined by the eigenstate. However, depending on the type of operator the potential is chosen to be, many distinct dynamics can be associated to the same fixed eigenstate. The nature of the stochastic processes associated with each reconstructed dynamic is also discussed, as well as a generalization of the stochastic dynamics formalism allowing for nonlocal potentials.

I. INTRODUCTION

Consider a Schrödinger operator $H = -\frac{1}{2}\Delta + V(x)$, where $V(x)$ is a multiplication operator, and a real function $\phi(x) \in L^2_{\text{loc}}(\mathbb{R}^n)$, such that $(-\frac{1}{2}\Delta + V - E)\phi = 0$. Let Ω be an open set in the support of the measure $d\nu = \phi^2\, dx$ and $\mathscr{H}_\nu(\Omega)$ the closed subspace of $L^2(\Omega, d\nu)$ obtained by closing $C_0^\infty(\Omega)$ in the $L^2(\Omega, d\nu)$ norm. For $f_1, f_2 \in C_0^1(\Omega)$, the quadratic form

$$\epsilon(f_1, f_2) = \frac{1}{2}\int \overline{\nabla f_1} \cdot \nabla f_2\, d\nu \tag{1.1}$$

is a local Markovian symmetric form on $L^2(\Omega, d\nu)$. If ϕ is such that the form ϵ is closable in $\mathscr{H}_\nu(\Omega)$ then its closure $\bar{\epsilon}$ is a local regular Dirichlet form.[1] Several closability conditions are known.[2–4] For example, $\phi > 0$ locally uniformly; $\phi = 0$ at most on a set of Lebesgue measure zero ($n = 1$) plus some regularity.

Conversely if $\bar{\epsilon}(f_1, f_2)$ is a densely defined symmetric positive closed form there is a positive self-adjoint operator H such that [2,5,6]

$$\bar{\epsilon}(f_1, f_2) = (H^{1/2} f_1, H^{1/2} f_2). \tag{1.2}$$

One has, therefore, a way to describe quantum dynamics through (energy) forms alternative to the conventional operator Schrödinger approach. In sufficiently well-behaved situations the two approaches are equivalent. In particular, if $\nabla\phi, \nabla\phi/\phi, \Delta\phi/\phi \in L^2_{\text{loc}}(\Omega)$, then $H = -\frac{1}{2}\Delta + V - E$ with

$$V - E = \tfrac{1}{2}\phi^{-1}\Delta\phi. \tag{1.3}$$

The Dirichlet approach is, however, more general in the sense that through regular Dirichlet forms one can describe dynamic situations which formally would correspond to potentials more singular than distributions.

The Dirichlet approach faces a uniqueness question, since $\epsilon(f_1, f_2) = \frac{1}{2}\int \overline{\nabla f_1}\cdot\nabla f_2\, d\nu$ is first defined on a dense domain, but for the characterization of quantum dynamics one needs a self-adjoint operator. In principle, distinct quantum dynamics would correspond to the possible nonequivalent extensions of ϵ. A certain number of uniqueness results are available, in particular when the operator associated with ϵ is essentially self-adjoint in $C_0^\infty(\Omega)$.[7,8]

In this paper, a different nonuniqueness question is discussed. This relates not to the equivalence of the Dirichlet and Schrödinger approaches as formulated above, but to the question of whether the ground state determines the dynamics uniquely.

The sense in which the eigenstate ϕ determines the dynamics is apparent in the potential equation (1.3) or in the fact that given, for example, $\phi \in L^2_{\text{loc}} \neq 0$ almost everywhere and $\nabla\phi \in L^2_{\text{loc}}(\mathbb{R}^n - N)$ (N a closed null set), then the form is closable and the positive self-adjoint operator H of Eq. (1.2) is unique. This uniqueness, however, is a consequence of the implicit assumption that V is a multiplication operator or equivalently that the energy form is the closure of a form of the type (1.1). Physically this assumption makes sense if one has grounds to believe in the assumed (canonical) decomposition of the Hamiltonian. This may be the case when reconstruction from the vacuum is used in models where the fundamental dynamic laws are presumed to be known, for example, lattice QED or QCD.[9]

In (nonrelativistic) many-body problems the situation may be quite different. In nuclear physics, for example, there is often more information on the nature of the ground state than on the form of the interaction potentials. It is also true that when the fundamental forces are known but many particles are in interaction, to determine experimentally without ambiguity the ground state structure may be easier than the effective one-body potential. Even when some parts of the potential correspond to known particle exchanges, it is only the leading static contribution that can be described by a multiplication potential. Higher-order contributions have a nonlocal nature.

When detailed information on the dynamic laws is lacking, a sensible question to address is the characterization of the possible dynamics compatible with a given (zero) energy eigenstate (or a finite set of known eigenstates). Defined in such a generality the question has infinitely many nonequivalent answers. One should somehow restrict the classes of operators one uses as candidate potentials.

In the Schrödinger and the Dirichlet approaches one

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deals, respectively, with the spaces $L^2(\mathbb{R}^n,dx)$ and $L^2(\mathbb{R}^n,d\nu)$, $d\nu=\phi^2dx$, the unitary map U_ϕ between them being multiplication by ϕ^{-1}:

$$g\in L^2(\mathbb{R}^n,dx)\xrightarrow{U_\phi} g\phi^{-1}\in L^2(\mathbb{R}^2,d\nu).$$

A natural restriction on the operators of the theory would be to require a simple operation on the product of functions, i.e., a multiplication law

$$V(g\phi)=F[g,\phi,Vg,V\phi]. \tag{1.4}$$

From linearity it follows that F is a homogeneous function of order 2. Linear operators with a multiplication law (1.4) are called Bourlet operators and have been studied extensively.[10,11]

Under fairly general conditions it can be shown that there are three types of Bourlet operators, namely multipliers V_M, derivations V_D, and substitution operators V_H. In $\mathbb{R}$, for example,

$$(V_Mg)(x)=\omega(x)g(x),$$

$$(V_Dg)(x)=\omega(x)\frac{d}{dx}g(x)-cg(x),$$

$$(V_Hg)(x)=(1/A)g[A\nu(x)]+\mu g(x).$$

Unfortunately, derivation and substitution operators are not symmetric in general and their symmetrized versions no longer obey the simple multiplication law (1.4). Therefore symmetrized derivation and substitution operators will be used, but we will not be restricted to these classes only.

The plan of the paper is the following: The potential V is considered to belong to one of the following operator classes: finite rank operators, second order (Sturm–Liouville) operators, symmetrized derivations, or symmetrized substitution operators. In each case, ϕ is considered to be a (zero-) energy eigenstate of the dynamics

$$(-\tfrac{1}{2}\Delta+V)\phi=0,$$

and V is determined in the assumed class. The nature of the (reconstructed) dynamics is then characterized by spectral analysis and (or) construction of the associated stochastic process through the Beurling–Deny formula. For explicit calculations and examples one concentrates on the one-dimensional case. As an illustrative example ϕ is taken to be the harmonic oscillator wave function $e^{-x^2/2}$. One finds in all operator classes distinct dynamics that contain this ϕ as a zero-energy eigenstate.

II. FINITE RANK POTENTIALS

An operator O is of finite rank if it can be written as

$$Of=\sum_{i=1}^{N}(g_i,f)h_i, \tag{2.1}$$

where $\{g_i,h_i\}$ are $2N$ vectors in a Hilbert space. Here one considers potentials that are sums of a constant with a symmetric finite rank operator

$$V_{RN}=c+\sum_{i,j=1}^{N}|h_i\rangle b_{ij}\langle h_j|, \tag{2.2}$$

where $b_{ij}^*=b_{ji}$ and c is a constant $\geqslant 0$. Let ϕ be a zero-energy eigenstate of $H_{RN}=-\frac{1}{2}\Delta+V_{RN}$. The state ϕ determines the potential uniquely only if $N=1$. Then one knows that

$$H_{R1}=-\tfrac{1}{2}\Delta+c-|h\rangle\langle h|=-\tfrac{1}{2}\Delta+V_{R1}, \tag{2.3a}$$

where

$$h=(\phi,(-\tfrac{1}{2}\Delta+c)\phi)^{-1/2}(-\tfrac{1}{2}\Delta+c)\phi. \tag{2.3b}$$

[For example if ϕ is the harmonic oscillator ground state $\phi\sim\exp(-x^2/2)$, then

$$h=\{(c+\tfrac{1}{4})u_0-\sqrt{2}/4u_2\}(c+\tfrac{1}{4})^{-1/2}, \tag{2.4}$$

where

$$u_n=(\sqrt{\pi}2^nn!)^{-1/2}H_n(x)e^{-x^2/2} \tag{2.5}$$

are the normalized eigenstates of the (multiplicative) harmonic oscillator.]

The spectral properties of a Hamiltonian H_{R1} with rank-one potential are known.[6,12] It has at most one eigenvector (bound state) and because the potential is a compact perturbation of $-\frac{1}{2}\Delta+c$ the continuous spectrum is $[c,\infty)$.

For the harmonic oscillator example, the corresponding (local) Hamiltonian with multiplicative potential is

$$H_M=-\frac{1}{2}\frac{d^2}{dx^2}+\frac{1}{2}(x^2-1).$$

Here H_M has a pure point spectrum $\{0,1,2,\ldots\}$, whereas the rank-one potential which has u_0 as a zero-energy eigenstate has very different spectral properties.

The basic qualitative difference between local (multiplicative) and finite rank potentials, even when they share one (or several) eigenvalues, becomes clearer if one examines the corresponding stochastic processes.

A local Hamiltonian with a zero-energy eigenstate $\phi(x)$ corresponds to a diffusion process with diffusion measure $\phi^2(x)d^nx$. To characterize the stochastic process associated with H_{R1}, one compares the (energy) form $\epsilon(f,g)=(f\phi,H_{R1}g\phi)$, f and g being real functions, with the Beurling–Deny formula

$$\begin{aligned}\epsilon(f,g)&=\frac{1}{2}\int\nabla f\cdot\nabla g\phi^2\,d^nx\\&\quad+\int f\phi\{V_{R1}(g\phi)-gV_{R1}\phi\}d^nx\\&=\frac{1}{2}\int\nabla f\cdot\nabla g\phi^2\,d^nx\\&\quad-\int f(x)\phi(x)h(x)\{g(y)\\&\quad-g(x)\}h(y)\phi(y)d^nx\,d^ny.\end{aligned} \tag{2.6}$$

For comparison purposes, one writes the Beurling–Deny formula

$$\begin{aligned}\epsilon(f,g)&=\int\partial_i f\,\partial_j g\mu_{ij}(dx)\\&\quad+\int(f(x)-f(y))(g(x)-g(y))\sigma(dx,dy)\\&\quad+\int f(x)g(x)k(dx)\end{aligned} \tag{2.7}$$

as follows:

$$\epsilon(f,g)=\int \partial_i f\,\partial_j g\,\mu_{ij}(x)dx + \int f(x)g(x)\left\{k(x)+2\int dy\,\sigma(x,y)\right\}dx - 2\int f(x)g(y)\sigma(x,y)dx\,dy, \tag{2.8}$$

where the measures are not necessarily absolutely continuous. Notice that when comparing Eq. (2.6) with (2.8), $\sigma(x,y)$ is defined only up to $\gamma(x)\,\delta(x-y)$, where $\gamma(x)$ is an arbitrary function. To obtain the actual jumping measure density one has to extract all terms proportional to $\delta(x-y)$.

Comparing (2.6) with (2.8) one concludes that the stochastic process associated with H_{R1} has diffusion, jumping, and killing measure densities, respectively,

$$\mu_{ij}(x)=\tfrac{1}{2}\phi^2(x)\delta_{ij}, \tag{2.9a}$$

$$\sigma(x,y)=\tfrac{1}{2}\phi(x)h(x)\phi(y)h(y), \tag{2.9b}$$

$$k(x)=0, \tag{2.9c}$$

with $h(x)$ a function of $\phi(x)$ [Eq. (2.3b)].

Intuitively, one might think that if one considered a rank N potential which coincided with a local potential in its action on N distinct functions, the jumping measure would vanish in the limit $N\to\infty$. This intuition turns out to be right only under particular conditions.

Let the Hamiltonian $H_N=H_0+\Sigma_{i,j=0}^{N-1}|i\rangle b_{ij}\langle j|$ share N eigenstates $\{\phi_i,\ i=0,\ldots,N-1\}$ with the local $H=H_0+V(x)$, i.e.,

$$H_N\phi_i=H\phi_i=E_i\phi_i. \tag{2.10}$$

Then it follows[13] that H_N has the form

$$H_N=H_0+\sum_{i,j=0}^{N-1}V|\phi_i\rangle(\mathscr{V}^{-1})_{ij}\langle\phi_j|V, \tag{2.11}$$

where $\mathscr{V}^{-1}$ is the inverse of the matrix $\mathscr{V}_{ij}=\langle\phi_i|V|\phi_j\rangle$. Comparing the energy form $\epsilon(f,g)=(f\phi_0,H_N g\phi_0)$ with the Beurling–Deny formula, as before, one obtains

$$\sigma(x,y)=-\frac{1}{2}\sum_{i,j=0}^{N-1}\phi_0(x)V(x)\phi_i(x)\times(\mathscr{V}^{-1})_{ij}\phi_j(y)V(y)\phi_0(y). \tag{2.12}$$

In the $N\to\infty$ limit the jumping disappears only if $\sigma(x,y)$ becomes proportional to $\delta(x-y)$,

$$\sum_{i,j=0}^{\infty}\phi_i(x)(\mathscr{V}^{-1})_{ij}\phi_j(y)\sim\delta(x-y) \tag{2.13}$$

(which holds if $\{\phi_i\}$ is a complete orthonormal set).

So far, the stochastic process associated with the Hamiltonian operator H has meant the Markov process with transition functions leading to the same semigroup as that generated by H. The Markov transition functions represent, therefore, the behavior of the Schrödinger equation in imaginary time.

Another connection between the Schrödinger equation and probabilistic notions is established in the framework of stochastic mechanics,[14] which concerns the time evolution of the probability density $\rho(x,t)=|\psi(x,t)|^2$ in real time. Consideration of nonlocal potentials requires an extension of the stochastic mechanics formalism, which is sketched below.

From the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi=-\frac{\hbar^2}{2m}\Delta\psi+V\psi \tag{2.14}$$

and its adjoint, one obtains

$$\frac{\partial\rho}{\partial t}=-\nabla\{b\rho\}+\frac{\hbar}{2m}\Delta\rho+\mathrm{Im}\int\Sigma(x,y)\rho(y,t)d^n y, \tag{2.15}$$

where

$$b=\frac{\hbar}{m}\nabla\ln|\psi|+\frac{\hbar}{m}\nabla\arg\psi=u+v, \tag{2.16a}$$

$$(V\psi)(x)=\int V(x,y)\psi(y)d^n y, \tag{2.16b}$$

$$\Sigma(x,y)=\frac{2}{\hbar}\psi^*(x,t)V(x,y)\frac{1}{\psi^*(y,t)}, \tag{2.16c}$$

and $V(x,y)=V^*(y,x)$. From (2.16a)–(2.16c), one sees that once a solution $\psi(x,t)$ of the Schrödinger equation is known, all parameters in (2.15) are known. However, one can interpret (2.15) as the forward equation of a stochastic process and use it, together with the equations of motion for u, v, and Σ, to define the dynamics without explicit reference to the Schrödinger equation. This is the point of view of stochastic mechanics.

The equations of motion for u, v, and Σ are

$$\dot u=-\frac{\hbar}{2m}\nabla_x(\nabla_x\cdot v)-\nabla_x(u\cdot v)-\frac{\hbar}{2m}\mathrm{Im}\,\nabla_x\int\Sigma(y,x)d^n y, \tag{2.17a}$$

$$\dot v=\frac{1}{2}\nabla_x(u^2-v^2)+\frac{\hbar}{2m}\nabla_x(\nabla_x\cdot u)-\frac{\hbar}{2m}\mathrm{Re}\,\nabla_x\int\Sigma(y,x)d^n y, \tag{2.17b}$$

$$\dot\Sigma(x,y)=\Sigma(x,y)\Big[\Big\{-\frac{m}{\hbar}u\cdot v(x)-\frac{1}{2}\nabla\cdot v(x)-\frac{im}{2\hbar}(u^2(x)-v^2(x))-\frac{i}{2}\nabla\cdot u(x)+\frac{i}{2}\int\Sigma(z,x)d^n z\Big\}-\{x\leftrightarrow y\}\Big]. \tag{2.17c}$$

In the local (multiplicative) operator case $V(x,y)=V(x)\delta(x-y)$ and the kernel Σ is

$$\Sigma_M(x,y)=(2/\hbar)V(x)\delta(x-y).$$

Then $\dot\Sigma_M(x,y)=0=\mathrm{Im}\,\Sigma_M(x,y)$ and the only contribution is the usual $(1/m)\nabla V(x)$, in the equation for $\dot v$.

For the case of the rank N potential of Eq. (2.2), the kernel has nontrivial dynamics. In terms of the solution of the Schrödinger equation, $\Sigma_{RN}(x,y)$ is

$$\Sigma_{RN}(x,y)=(2/\hbar)c\delta(x-y)+\frac{2}{\hbar}\sum_{i,j=1}^{N}\psi^*(x,t)h_i(x)b_{ij}h_j^*(y)\frac{1}{\psi^*(y,t)}. \tag{2.18}$$

III. STURM–LIOUVILLE POTENTIAL

Let the potential be a second-order differential operator with real coefficients. Symmetry restricts the operator to the general form

$$V_{\rm SL} = -K^{ij}(x)\frac{\partial^2}{\partial x^i\,\partial x^j} - \left(\frac{\partial}{\partial x^i}K^{ij}(x)\right)\frac{\partial}{\partial x^j} + G(x), \tag{3.1}$$

with $K^{ij}(x) = K^{ji}(x)$. This is called a Sturm–Liouville operator. Some of the nonlocal potentials used in nuclear physics[15,16] are of this type.

Of particular interest are the one-dimensional and the spherically symmetric three-dimensional cases. In three dimensions, with spherical symmetry $K^{ij}(x) = K(r)\delta^{ij}$, $G(x) = G(r)$, and writing the wave function as

$$\psi(r,\theta,\phi) = (u(r)/r)Y_{lm}(\theta,\phi),$$

one obtains for the radial eigenvalue equation

$$\left\{\left(\frac{1}{2}+K(r)\right)\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}\right) - \frac{dK}{dr}\frac{d}{dr} + \frac{1}{r}\frac{dK}{dr} + G(r) - E\right\}u(r) = 0. \tag{3.2}$$

As before $\hbar = m = 1$, for simplicity, otherwise the factor $\frac{1}{2} + K(r)$ should be replaced by $\hbar^2/2m + K(r)$.

Let ϕ be a zero-energy eigenvalue

$$H_{\rm SL}\phi = (-\tfrac{1}{2}\Delta + V_{\rm SL})\phi = 0. \tag{3.3}$$

Using (3.3) to compute the energy form $\epsilon(f,g)$ one obtains

$$\epsilon(f,g) = (f\phi, H_{\rm SL}g\phi) = \int \partial_i f\left\{\frac{1}{2}\delta^{ij} + K^{ij}(x)\right\}\partial_j g\,\phi^2\,d^n x. \tag{3.4}$$

Hence, in the Sturm–Liouville case, the associated stochastic process is (as in the multiplication potential case) a pure diffusion with a (modified) diffusion measure density

$$\mu_{ij}(x) = \{\tfrac{1}{2}\delta^{ij} + K^{ij}(x)\}\phi^2(x). \tag{3.5}$$

This refers to the stochastic process associated with the imaginary time Schrödinger equation. In real time, the equation of motion for the probability density $\rho(x,t) = |\phi(x,t)|^2$, Eq. (2.15), is in this case

$$\frac{\partial\rho}{\partial t} = -\partial_i\{b^i\rho\} + \partial_i\{\nu^{ij}(x)\partial_j\rho\}, \tag{3.6}$$

with

$$b^i = \frac{2}{\hbar}\left(\frac{\hbar^2}{2m}\delta^{ij} + K^{ij}(x)\right)(\partial_j \arg\psi + \partial_j \ln|\psi|) \tag{3.7a}$$

$$\nu^{ij} = \frac{1}{\hbar}\left(\frac{\hbar^2}{2m}\delta^{ij} + K^{ij}(x)\right), \tag{3.7b}$$

i.e., a generalized Fokker–Planck equation with a space dependent diffusion.

Nonlocalities of the Sturm–Liouville type are relatively mild in the sense that the stochastic processes associated with imaginary time evolution and with the stochastic mechanics description are both generalized diffusions.

Nonlocal potentials of the type studied in this section can be transformed to a form which may be handled by the same computational techniques as local potentials. For the one-dimensional (or the radial) equation one performs the transformation[17]

$$\psi = (\tfrac{1}{2} + K)^{-1/2}\chi \tag{3.8}$$

in

$$\left\{-\left(\frac{1}{2}+K\right)\frac{d^2}{dx^2} - K'\frac{d}{dx}\right\}\psi + G\psi = E\psi \tag{3.9}$$

to obtain

$$-\chi'' + \left\{\left(G + \frac{K''}{2} - E\right)\left(\frac{1}{2}+K\right)^{-1} - \frac{K'^2}{4}\left(\frac{1}{2}+K\right)^{-2}\right\}\chi = 0. \tag{3.10}$$

The nonlocal eigenvalue problem is therefore transformed into the search for the zero-energy eigenvalue of a local energy-dependent potential.

The requirement (3.3) that ϕ be a zero-energy eigenstate leads to an equation

$$\partial_j\phi\,\partial_i K^{ij} + \partial_i\,\partial_j\phi K^{ij} = G\phi - \tfrac{1}{2}\Delta\phi, \tag{3.11}$$

which for each ϕ, determines $G(x)$ once $K^{ij}(x)$ is fixed, or conversely.

To learn about the nature of the dynamics that are reconstructed when nonlocalities of the Sturm–Liouville type are chosen, one analyzes briefly the one-dimensional case.

Let ϕ be the harmonic oscillator ground state $\exp\{-x^2/2\}$.

When $K(x)$ is a constant (K) the coefficient of d/dx in (3.1) vanishes and $H_{\rm SL}$ with $G(x)$ obtained from (3.11) is simply the Hamiltonian of a harmonic oscillator multiplied by the factor $(1 + 2K)$. The eigenstates are the same, with the scale factor $(1 + 2K)$ multiplying the eigenvalues.

A nonconstant $K(x)$ may be interpreted as a description of space inhomogeneity of the oscillator parameters. Defining

$$m(x) = (1 + 2K(x))^{-1}, \tag{3.12}$$

one rewrites Eq. (3.9) as

$$\left\{-\frac{1}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{1}{dx}\right) + G(x)\right\}\psi = E\psi, \tag{3.13}$$

which can be interpreted as describing the motion of a variable mass particle in the potential $G(x)$. However, if dm/dx is large this intuitive interpretation may be misleading because the contribution of the derivative terms may become more important than the static potential $G(x)$.

With the same zero-energy eigenstate, one can associate very many distinct Sturm–Liouville operators. For example both

$$K = x^2;\quad G = x^4 - \tfrac{5}{2}x^2 - \tfrac{1}{2} \tag{3.14}$$

and

$$K = \tfrac{1}{2}(e^{x^2} - 1);\quad G = -\tfrac{1}{2}(x^2 + 1)e^{x^2} \tag{3.15}$$

have $\phi = e^{-x^2/2}$ as a zero-energy eigenstate, although their static potentials are quite different. In (3.14) it is a double well, whereas in (3.15) the static potential is not bounded from below. However, in (3.15) the derivative part of the potential is sufficiently strong to overcome the static negative unbounded contribution. In particular it is easy to prove

that the negative real axis belongs to the resolvent set.

The Hamiltonian operator associated with the choice (3.15) is

$$H_{\rm SL} = -\frac{1}{2}e^{x^2}\left(x+\frac{d}{dx}\right)^2 = -\frac{1}{2}e^{x^2/2}\frac{d^2}{dx^2}e^{x^2/2}. \quad (3.16)$$

This operator is, at least from a mathematical point of view, sufficiently interesting to deserve further study. $H_{\rm SL}$ is symmetric in $C_0^\infty(\mathbb{R})$ and commutes with complex conjugation. By von Neumann's theorem[18] it has self-adjoint extensions, which one characterizes by specifying the boundary conditions at $\pm\infty$. From

$$\int \psi_2^* H_{\rm SL}\psi_1\,dx = \int (H_{\rm SL}\psi_2)^*\psi_1\,dx - \frac{1}{2}e^{x^2/2}\left\{\psi_2^*\frac{d}{dx}(e^{x^2/2}\psi_1) - \frac{d}{dx}(e^{x^2/2}\psi_2)^*\psi_1\right\}\Big|_{-\infty}^{\infty}$$

one is led to define the following domain for the self-adjoint extensions:

$$D(H_{\rm SL}^{(\theta)}) = \Big\{\psi\in L^2 \,|\, H_{\rm SL}\psi\in L^2;\ \lim_{x\to\infty} e^{x^2/2}\psi = e^{i\theta}\lim_{x\to-\infty} e^{x^2/2}\psi,\ \lim_{x\to\infty}\frac{d}{dx}(e^{x^2/2}\psi) = e^{i\theta}\lim_{x\to-\infty}\frac{d}{dx}(e^{x^2/2}\psi)\Big\}. \quad (3.17)$$

Requiring $\phi = e^{-x^2/2}$ to be an eigenstate one is led to choose the self-adjoint extension $H_{\rm SL}^{(0)}$. Notice that $H_{\rm SL}$ has a two-dimensional subspace of zero energy eigenstates, namely $(c_1x+c_2)e^{-x^2/2}$. The choice of a particular self-adjoint extension selects one vector in this subspace.

The negative real axis belongs to the resolvent set of $H_{\rm SL}^{(0)}$ and there is a point spectrum contained in $[0,\infty)$. This analysis is divided into two parts.

A. $\forall\lambda<0, \lambda\notin\sigma(H_{\rm SL}^{(0)})$

According to Weyl's criterion $\lambda\in\sigma(H_{\rm SL}^{(0)})$ if and only if there is a sequence ψ_n in $D(H_{\rm SL}^{(0)})$, with $\|\psi_n\|=1$, such that $\lim_{n\to\infty}\|(H_{\rm SL}^{(0)}-\lambda)\psi_n\|=0$.

Defining

$$\psi_n = e^{-x^2/2}\gamma_n, \quad (3.18)$$

and using the boundary conditions in $D(H_{\rm SL}^{(0)})$ to perform the partial integrations, one obtains

$$\|(H_{\rm SL}^{(0)}-\lambda)\psi_n\|^2 = \int dx\left\{\frac{e^{x^2}}{4}|\gamma_n''|^2 - \lambda|\gamma_n'|^2 + \lambda^2 e^{-x^2}|\gamma_n|^2\right\}.$$

If $\lambda<0$, the right-hand side is a sum of positive quantities and is $\neq 0$ because

$$\int dx\, e^{-x^2}|\gamma_n|^2 = \|\psi_n\| = 1.$$

Therefore any $\lambda<0$ belongs to the resolvent set of $H_{\rm SL}^{(0)}$.

B. $\lambda\geqslant 0$

Using (3.18) one writes

$$(H_{\rm SL}^{(0)}-\lambda)\psi_n = e^{x^2/2}\left\{-\frac{1}{2}\frac{d^2}{dx^2}-\lambda e^{-x^2}\right\}\gamma_n. \quad (3.19)$$

The question of whether λ belongs to the spectrum of $H_{\rm SL}^{(0)}$ is therefore related to the zero eigenvalue problem for the operator

$$B_\lambda = -\frac{1}{2}\frac{d^2}{dx^2}-\lambda e^{-x^2}.$$

Because λe^{-x^2} is an L^2 perturbation, $\sigma_{\rm ess}(B_\lambda) = \sigma_{\rm ess}(-d^2/dx^2)$, which implies $0\in\sigma(B_\lambda)$. Because zero is in the spectrum of B_λ, there is a sequence γ_n with $\|\gamma_n\|=1$ such that $\|B_\lambda\gamma_n\|\to 0$. However this does not guarantee that $\|e^{x^2/2}B_\lambda\gamma_n\|\to 0$, nor that $\|e^{-x^2/2}\gamma_n\|$ remains $\neq 0$ in the $n\to\infty$ limit.

Instead, one analyzes directly the equation

$$\left\{\frac{d^2}{dx^2}+2\lambda e^{-x^2}\right\}\gamma(x)=0. \quad (3.20)$$

In a neighborhood of $\pm\infty$, this equation has an asymptotic solution $\alpha_\pm x+\beta_\pm$. If one requires that $\psi = e^{-x^2/2}\gamma\in D(H_{\rm SL}^{(0)})$, then $\alpha_\pm=0$ and $\beta_+=\beta_-$.

Fix $\gamma\to\beta_-$ and $\gamma'\to 0$ when $x\to-\infty$ as initial conditions. Because e^{-x^2} is continuous in $(-\infty,\infty)$ the existence–uniqueness theorem for second-order linear homogeneous equations[19] implies, for any λ, the existence of a solution to (3.20), which at $x\to+\infty$ grows at most linearly. Therefore, the problem $(H_{\rm SL}^{(0)}-\lambda)\psi=0$ has an L^2 solutions for any λ. This does not imply that all λ's are in the spectrum because in general ψ will not belong to the domain $D(H_{\rm SL}^{(0)})$. ψ is in $D(H_{\rm SL}^{(0)})$ only if $\lim_{x\to\infty}\gamma(x)=\beta_-$. The λ values for which this condition holds are the elements of the point spectrum of $H_{\rm SL}^{(0)}$. Below, the first seven such values obtained by numerical integration of (3.20) are listed:

0 4.33 15.07 32.14

55.52 85.21 121.19 ...

Qualitatively they follow the same pattern as $\lambda\sim\pi n^2$, which is obtained from the semiclassical approximation

$$\gamma(x)\sim\cos\int_{-\infty}^{x}\sqrt{2\lambda}\,e^{-\eta^2/2}d\eta.$$

IV. SYMMETRIZED DERIVATION

The potential that is to be studied in this section is required to have the form

$$V_D = \left\{a(x), i\frac{\partial}{\partial x}\right\}_+ + W(x) = 2ia(x)\frac{\partial}{\partial x} + i\frac{da}{dx} + W(x), \quad (4.1)$$

where $a(x)$ and $W(x)$ are real functions in $\mathbb{R}$.

Let $\phi(x)$ be a real zero energy eigenstate

$$H_D\phi = \left(-\frac{1}{2}\frac{d^2}{dx^2}+V_D\right)\phi = 0.$$

Then one obtains

$$a(x) = (c/2)\phi^{-2}(x), \tag{4.2a}$$

$$W(x) = \frac{1}{2\phi(x)}\frac{d^2\phi}{dx^2}, \tag{4.2b}$$

c being an arbitrary constant. For the harmonic oscillator ground state $\phi = e^{-x^2/2}$,

$$V_D = \frac{c}{2}\left\{e^{x^2}, i\frac{\partial}{\partial x}\right\}_+ + \frac{1}{2}(x^2-1)$$
$$= cie^{x^2}\left(x + \frac{d}{dx}\right) + \frac{1}{2}(x^2-1). \tag{4.3}$$

Even when c is small the term $c[e^{x^2}, i(\partial/\partial x)]_+$ cannot be considered a perturbation of the (multiplicative) harmonic oscillator, because the operator V'

$$V' = ie^{x^2}\left(x + \frac{\partial}{\partial x}\right) = e^{x^2/2} i\frac{d}{dx} e^{x^2/2} \tag{4.4}$$

has divergent matrix elements in the $\{u_n\}$ basis. More precisely, except for u_0 all other u_n's are not in the domain of V':

$$V'u_n = ie^{x^2}\sqrt{2n}\,u_{n-1} \notin L^2(\mathbb{R}), \quad \text{if } n \neq 0.$$

The operator $H_D = -\frac{1}{2}(d^2/dx^2) + V_D$ is symmetric in $C_0^\infty(\mathbb{R})$ and unitarily equivalent (see below) to a real potential. It has a one-parameter family of self-adjoint extensions which one characterizes by the boundary conditions at $\pm\infty$. From

$$\int \psi_2^* ie^{x^2}\left(x + \frac{d}{dx}\right)\psi_1\, dx$$
$$= i\psi_2^* e^{x^2}\psi_1\Big|_{\infty}^{-\infty} + \int\left[ie^{x^2}\left(x + \frac{d}{dx}\right)\psi_2\right]^*\psi_1\, dx$$

one obtains the following domains for the self-adjoint extensions

$$D(H_D^{(\theta)}) = \{\psi \in L^2 | H_D\psi \in L^2,$$

$$\lim_{x\to\infty} e^{x^2/2}\psi = e^{i\theta}\lim_{x\to-\infty} e^{x^2/2}\psi\}. \tag{4.5}$$

The self-adjoint extension that contains $e^{-x^2/2}$ in its domain, as required, is $H_D^{(0)}$. Although it shares this zero energy eigenstate with the harmonic oscillator, the dynamic is otherwise of a completely different nature. This becomes apparent if one considers the isometric map

$$\psi(x) \to (U_c\psi)(x) = \exp\left\{-ic\int_0^x e^{\xi^2}\, d\xi\right\}\psi(x). \tag{4.6}$$

Then

$$H' = U_c H_D U_c^{-1} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x^2-1) - \frac{c^2}{2}e^{2x^2} \tag{4.7}$$

is the harmonic oscillator Hamiltonian plus a negative unbounded potential.

To H_D is associated a singular jumping measure. Computing the energy form $\epsilon(f,g) = (f\phi, H_D g\phi)$ and comparison with the Beurling–Deny formula as in (2.6)–(2.8) leads to

$$\mu_{ij}(x) = \tfrac{1}{2}\phi^2(x)\delta_{ij}, \tag{4.8a}$$

$$\sigma(x,y) = (-ic/2)\delta'(x-y), \tag{4.8b}$$

$$k(x) = 0. \tag{4.8c}$$

The kernel $\Sigma_D(x,y)$ for the stochastic mechanics equation (2.15) is

$$\Sigma_D(x,y) = \frac{2}{\hbar}\left\{W(x) + i\frac{da}{dx} - 2ia(x)\frac{d}{dx}\ln\psi^*(x)\right\}\delta(x-y)$$
$$+ \frac{4}{\hbar}ia(x)\delta'(x-y). \tag{4.9}$$

V. POTENTIALS WITH SUBSTITUTION OPERATORS

Symmetrized substitution operators may also be of some interest in the description of effective nuclear interactions.[20] They have the general form

$$(V_s\psi)(x) = \frac{1}{\omega(x)}\psi(\nu(x))$$
$$+ \frac{1}{\omega^*(\nu^{-1}(x))}\left(\frac{d\nu^{-1}}{dx}\right)^*\psi(\nu^{-1}(x)) + q(x)\psi(x). \tag{5.1}$$

Using $H_s\phi = (-\frac{1}{2}\Delta + V_s)\phi = 0$ one can, as before, compute the energy form $\epsilon(f,g) = (f\phi, H_s g\phi)$ and compare with the Beurling–Deny formula to obtain for the diffusion, jumping, and killing

$$\mu_{ij}(x) = \tfrac{1}{2}\phi^2(x)\delta_{ij}, \tag{5.2a}$$

$$\sigma(x) = -\frac{1}{2}\left\{\frac{1}{\omega(x)}\delta(y - \nu(x))\right.$$
$$\left. + \frac{1}{\omega^*(y)}\left(\frac{d\nu^{-1}}{dx}\right)^*\delta(y - \nu^{-1}(x))\right\}\phi(x)\phi(y), \tag{5.2b}$$

$$k(x) = 0. \tag{5.2c}$$

Example: Let $\phi = e^{-x^2/2}, \omega(x) = 1$, and the substitution function be a translation $\nu(x) = x + b$.

Then

$$q(x) = \tfrac{1}{2}(x^2-1) - 2e^{-b^2/2}\cosh bx. \tag{5.3}$$

Because the translation operators can be written in differential form, the Hamiltonian is

$$H_s = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x^2-1) + 2\cosh\left(b\frac{d}{dx}\right)$$
$$- 2e^{-b^2/2}\cosh bx. \tag{5.4}$$

From the fact that $H_s u_n \in L^2$ it follows that, in principle and for small b, the two last terms in (5.4) can be treated as a perturbation. From

$$H_s = (1-2b^2)\left\{-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x^2-1)\right\} + O(b^4),$$

one concludes that in leading order the effect of the perturbation is a scale change in the harmonic oscillator spectrum.

VI. RECONSTRUCTION FROM A STOCHASTIC PROCESS

If $\epsilon(f,g)$ is a closed positive symmetric form densely defined in $L^2(\Omega, d\mu)$ ($\Omega \subset \mathbb{R}^n$ open) there is a unique self-adjoint operator $\hat{H}$ such that $\epsilon(f,g) = (\hat{H}^{1/2}f, \hat{H}^{1/2}g)_{d\mu}$, where $(\cdot)_{d\mu}$ is the scalar product in $L^2(\Omega, d\mu)$. Here one is concerned not with $\hat{H}$ but with the operator H in the corresponding Schrö-

dinger form. Given a (Dirichlet) form by its measure densities, H is an operator such that

$$\epsilon(f,g) = (f,\hat{H}g)_{d\mu} = (\psi_f, H\psi_g)_{dx}, \tag{6.1}$$

where dx denotes the "flat" Lebesgue measure, and ψ_f, ψ_g are related to f,g by unitary equivalence.

Let ϵ be defined as in (2.7) by the measure densities $\mu_{ij}(x)$, $\sigma(x,y)$, $k(x)$, and

$$H = -\tfrac{1}{2}\Delta + V. \tag{6.2}$$

Assume that $\mu_{ij}(x) = \mu(x)\delta_{ij}$ and $\mu(x) > 0$ everywhere. The states in $L^2(\Omega,d\mu)$ and $L^2(\Omega,dx)$ are related by

$$f \xrightarrow{U_\mu} \psi_f = f\sqrt{2\mu}, \tag{6.3}$$

thus one obtains by a straightforward calculation using (6.1) and (2.8)

$$(V(\mu,\sigma,k)\psi)(x) = \left[\frac{1}{2}\frac{\Delta\sqrt{2\mu(x)}}{\sqrt{\mu(x)}} + \frac{1}{2\mu(x)}\left\{k(x) + 2\int \sigma(x,y)d^n y\right\}\right]\psi(x) - \int \frac{\sigma(x,y)}{\sqrt{\mu(x)\mu(y)}}\psi(y)d^n y. \tag{6.4}$$

From (6.4) it would seem that nonlocal potential effects can only be associated to the jumping measure. However one should notice that the potential in (6.2) is not uniquely defined, it depends on the choice of the unitary transformation U between $L^2(\Omega,d\mu)$ and $L^2(\Omega,dx)$. Let us decompose $\mu(x) = \alpha(x) + \beta(x)$ where now one requires only $\alpha(x) > 0$. Using now

$$f \xrightarrow{U_\alpha} \psi_f = f\sqrt{2\alpha}, \tag{6.5}$$

one obtains for the potential in (6.2)

$$V = V(\alpha,\sigma,k) - \frac{\beta}{2\alpha}\Delta - \nabla\left(\frac{\beta}{2\alpha}\right)\cdot\nabla - \frac{1}{\sqrt{2\alpha}}\nabla\cdot\left(\beta\nabla\frac{1}{\sqrt{2\alpha}}\right). \tag{6.6}$$

The nonlocal part in (6.6) that is not related to the jumping measure is of the Sturm–Liouville type.

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