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Explicit time-dependent Schrödinger propagators

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Abstract. We compute explicitly the time-dependent Schrödinger and heat propagator for the potentials $-[\lambda^2 m(m+1)]/\cosh^2 \lambda x$, a δ function potential, several cases of periodic δ function potentials and a δ function potential in a square well. We also discuss the semiclassical approximation for the δ function potential.

1. Introduction

There are few *time-dependent* Schrödinger propagators that can be computed explicitly. Except for the case of quadratic Hamiltonians [1, 2] (which includes the harmonic oscillators with constant electric or magnetic field) where the path integral can be done exactly and is equal to its semiclassical approximation, or for systems which are in some sense free [2], we know only the example of the knife edge [3, 4] and the case of reflectionless potentials [5, 6]; in all these cases, the propagator is a superposition of Gaussians. Note that we distinguish the time-dependent propagator from the energy-dependent Green function for which many more explicit examples are known [7, 8, 9].

The object of this paper is to compute three other examples of time-dependent propagators: the first is the $\cosh^{-2} x$ potential (also studied in [5]; however, our method is different); the second one is the δ function potential which can be done both by functional integrals and by spectral resolution; the third set of examples are various combinations of δ potentials, two cases of periodic δ potential and a δ potential in a square well.

In principle, one can recover the time-dependent propagator by Fourier transforming the energy-dependent propagator but this may not be very explicit; for example, the $\cosh^{-2} x$ potential has a very simple time-dependent propagator, but a complicated energy propagator (see [8]); the same remark applies to some cases of δ function potentials for which the energy-dependent propagators have been computed in various situations (see [7] for general information on δ function potentials).

One of the reasons why it is important to obtain a simple expression for time-dependent propagators is the study of non-stationary problems in quantum mechanics. In particular, the influence of an external random environment depending on time and the relation between quantum dissipation and tunnelling can be satisfactorily handled only if we know the time-dependent propagators of the non-perturbed problems.

2. The potential $\cosh^{-2} x$

We start with a general remark. Suppose that one can solve both the heat equation

$$\partial^2 v/\partial x^2 = \varphi v + \partial v/\partial t \tag{2.1}$$

and the eigenvalue problem

$$\partial^2 f/\partial x^2 = \varphi f + h_1 f \tag{2.2}$$

where φ is a given function of x and h_1 a given constant. We define

$$u(x, t) = \partial v(x, t)/\partial x - v(x, t) f^{-1}(x) \partial f(x)/\partial x. \tag{2.3}$$

A direct calculation shows that u satisfies the heat equation

$$\frac{\partial^2 u}{\partial x^2} = -\left[f^{-1} \frac{\partial^2 f}{\partial x^2} - 2f^{-2}\left(\frac{\partial f}{\partial x}\right)^2 + h_1 \right] u + \frac{\partial u}{\partial t}. \tag{2.4}$$

This procedure is analogous to the identity employed by Darboux [10] for eigenvalue problems.

Suppose now that we want to solve the initial value problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \left[h_1 + f^{-1} \frac{\partial^2 f}{\partial x^2} - 2f^{-2}\left(\frac{\partial f}{\partial x}\right)^2 \right] u \qquad u|_{t=0} = u_0. \tag{2.5}$$

First return to equation (2.1), defining $v_0(x)$ by

$$u_0(x) = \partial v_0/\partial x - v_0 f^{-1} \partial f/\partial x.$$

Thus

$$v_0(x) = f(x) \int_\alpha^x \frac{u_0(x')}{f(x')} \mathrm{d}x'. \tag{2.6}$$

We then consider the initial value problem

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} - \varphi v \qquad v|_{t=0} = v_0. \tag{2.7}$$

Our assumption is that we can solve (2.7) explicitly by a function $v(t, x)$. We return to (2.5) by the formula

$$u(t, x) = \partial v/\partial x - v f^{-1} \partial f/\partial x. \tag{2.8}$$

It is clear, by our previous calculations, that it solves (2.5) and that it is u_0 at $t = 0$. We apply this method to the case

$$f(x) = \cosh^{-\beta} \lambda x.$$

Then

$$\frac{\partial^2 f}{\partial x^2} = \frac{\beta^2 \lambda^2}{\cosh^\beta \lambda x} - \frac{\beta(\beta+1)\lambda^2}{\cosh^{\beta+2} \lambda x}.$$

Fix an integer m and choose $\beta = -(m+1)$, then

$$\frac{\partial^2 f}{\partial x^2} = -\frac{m(m+1)\lambda^2}{\cosh^2 \lambda x} f + [(m+1)\lambda]^2 f. \tag{2.9}$$

Define

$$\varphi_{m+1} = -\frac{\lambda^2 m(m+1)}{\cosh^2 \lambda x}$$

$$f_{m+1} = \cosh^{m+1} \lambda x$$

$$h_{m+1} = [(m+1)\lambda]^2.$$

If we can solve

$$\partial v/\partial t = \partial^2 v/\partial x^2 - \varphi_{m+1} v \tag{2.10$_{m+1}$}$$

then the function u

$$u = \partial v/\partial t - v(m+1)\lambda \tanh \lambda x \tag{2.11$_{m+1}$}$$

satisfies (2.5) with f_{m+1} and h_{m+1}:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \left[h_{m+1} + f_{m+1}^{-1} \frac{\partial^2 f_{m+1}}{\partial x^2} - 2f_{m+1}^{-2} \left(\frac{\partial f_{m+1}}{\partial x} \right)^2 \right] u. \tag{2.12}$$

The term in square brackets in (2.12) is exactly

$$\frac{(m+1)(m+2)\lambda^2}{\cosh^2 \lambda x} \equiv -\varphi_{m+2}(x)$$

so that if we can solve $(2.10)_{m+1}$, we can also solve $(2.10)_{m+2}$ by the transformation $(2.11)_{m+1}$.

Suppose, for example, that we want to solve

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{2\lambda^2}{\cosh^2 x} u \qquad u|_{t=0} = u_0 . \tag{2.13}$$

Call $G_0(x - x_0, t)$ the free propagator of

$$\partial v/\partial t = \partial^2 v/\partial x^2 \qquad v|_{t=0} = v_0 . \tag{2.14}$$

We start with (2.6) and define

$$v_0(x) = \cosh \lambda x \int_\alpha^x \frac{u_0(x')}{\cosh \lambda x'} \, dx'$$

then solve (2.14) by

$$v(t, x) = \int G_0(x - x_0, t) v_0(x_0) \, dx_0$$

and apply (2.6) to obtain

$$u(t, x) = \frac{\partial}{\partial x} \left[\int G_0(x - x_0, t) \cosh \lambda x_0 \left(\int_\alpha^{x_0} \frac{u_0(x')}{\cosh \lambda x'} \, dx' \right) dx_0 \right]$$
$$- \lambda \tanh \lambda x \int G_0(x - x_0, t) \cosh \lambda x_0 \left(\int_\alpha^{x_0} \frac{u_0(x') \, dx'}{\cosh \lambda x'} \right) dx_0 .$$

This does not depend on the choice of α and integrating by parts using $\alpha=-\infty$, we obtain

$$u(t,x)=\int \mathrm{d}x'\, u_0(x')\bigg[G_0(x-x',t)+\lambda\bigg(\int_{x'-x}^{+\infty} G_0(y,t)\sinh\lambda y\,\mathrm{d}y\bigg)(\cosh\lambda x\cosh\lambda x')^{-1}\bigg] \tag{2.15}$$

which is equivalent to Crandall's expression [5]. This formula gives the kernel $P_t^{(2)}(x,x')$ of equation $(2.10)_2$.

Denote in general by $P_t^{(m+1)}(x,x')$ the propagator for $(2.10)_{m+1}$; we can obtain the propagator of equation $(2.10)_{m+2}$

$$P_t^{(m+2)}(x,x')=\frac{1}{\cosh^{m+1}\lambda x'}\bigg(\frac{\partial}{\partial x}-\lambda(m+1)\tanh\lambda x\bigg)\times\bigg(\int_{x'}^{+\infty} P_t^{(m+1)}(x,\xi)\cosh^{m+1}\lambda\xi\,\mathrm{d}\xi\bigg). \tag{2.16}$$

The Schrödinger propagator is obtained by changing t into $\mathrm{i}t$ in these formulae.

3. The potential $\delta(x)$: propagating $H=-\frac{1}{2}(\partial^2/\partial x^2)-a\delta(x)$

3.1. *Using functional integrals*

We first recall some facts about standard Brownian motion [11, 12]. Call b_t the Brownian path starting at $t=0$ from $x=0$. The reflected Brownian path is $|b_t|$ and its local time spent at $x=0$ up to time t is

$$\tau(t)=\lim_{\varepsilon\to 0}\frac{1}{2\varepsilon}\int_0^t \chi_{[0,+\varepsilon]}(|b_s|)\,\mathrm{d}s \tag{3.1}$$

where $\chi_{[0+\varepsilon]}$ is the characteristic function of the set $[0,+\varepsilon]$; this random variable exists by a theorem of Levy [12, p 68].

Now, there is another way to describe the reflected Brownian motion and its local time. Let

$$X(t)=-b_t+\max_{0\le s\le t} b_s$$
$$\theta(t)=\max_{0\le s\le t} b_s. \tag{3.2}$$

It is known that the process $(X(t),\theta(t))$ has the same joint laws as the process $(|b_t|,\tau(t))$ defined above (see [11] or [12]).

Suppose now we consider the initial value problem

$$\partial u/\partial t=\tfrac{1}{2}\partial^2 u/\partial x^2+a\delta(x)u \qquad u|_{t=0}=u_0. \tag{3.3}$$

We approach this problem by the following:

$$\partial u_\varepsilon/\partial t=\tfrac{1}{2}\partial u_\varepsilon/\partial x^2+(a/2\varepsilon)\chi_{[-\varepsilon,\varepsilon]}(x)u_\varepsilon \qquad u_\varepsilon|_{t=0}=u_0. \tag{3.3$_\varepsilon$}$$

For problem $(3.3)_\varepsilon$ we have a probabilistic solution by the Feynman-Kac formula

$$u_\varepsilon(t, x) = E\left[\exp\left(\frac{a}{2\varepsilon}\int_0^t \chi_{[-\varepsilon,\varepsilon]}(x+b_s)\,\mathrm{d}s\right)u_0(x+b_t)\right]. \tag{3.4}$$

Suppose now that we start at time $t=0$ from $x=0$. The corresponding propagator is

$$K_\varepsilon(x', t\,|\,0) = E\left[\exp\left(\frac{a}{2\varepsilon}\int_0^t \chi_{[-\varepsilon,\varepsilon]}(b_s)\,\mathrm{d}s\right)\chi(b_t \in \mathrm{d}x')\right].$$

It is clear that this depends only on $|x|$ and if $a<0$, by Lebesgue theorem, this tends to

$$K(x', t\,|\,0)\,\mathrm{d}x' = \tfrac{1}{2}E_0(\exp(a\tau(t))\chi(|b_t| \in \mathrm{d}x')).$$

However, by the previous remark, this is

$$K(x', t\,|\,0)\,\mathrm{d}x' \equiv \tfrac{1}{2}E_0\left(\exp\left(a \max_{s\leq t} b_s\right)\chi\left(-b_t + \max_{s\leq t} b_s \in \mathrm{d}x'\right)\right).$$

Now by McKean [12, p 27], it is known that

$$\mathrm{Prob}\left(b_t \in \mathrm{d}x, \max_{s\leq t} b_s \in \mathrm{d}y\right) = \left(\frac{2}{\pi t^3}\right)^{1/2}(2y-x)\exp-\left(\frac{(2y-x)^2}{2t}\right)\chi(y>x)\,\mathrm{d}y\,\mathrm{d}x$$

and so

$$K(x, t\,|\,0)\,\mathrm{d}x = \left[\int_0^{+\infty} \mathrm{e}^{a\tau}\left(\frac{2}{\pi t^3}\right)^{1/2}(\tau+x)\exp[-(\tau+x)^2/2t]\,\mathrm{d}\tau\right]\mathrm{d}x$$

and after a slight transformation we obtain

$$K(x, t\,|\,0) = \frac{1}{(2\pi t)^{1/2}}\exp(-x^2/2t) + \frac{a}{(2\pi t)^{1/2}}\int_0^{+\infty} \mathrm{e}^{+a\xi}\exp[-(\xi+|x|)^2/2t]\,\mathrm{d}\xi. \tag{3.5}$$

This formula has been derived rigorously if $a \leq 0$. However we can continue it to $a>0$ also, because the integral is still absolutely convergent.

Next we obtain the propagator starting from any x_0. Consider the Brownian path starting from x_0

$$K(x, t\,|\,x_0)\,\mathrm{d}x = E(\exp(a\tau(t))\chi(x_0+b_t \in \mathrm{d}x)).$$

We call T_0 the first hitting time of point 0.

For $t<T_0$, $\tau(t)=0$ obviously. Using the Markov property we obtain

$$\begin{aligned} K(x, t\,|\,x_0)\,\mathrm{d}x &= E_{x_0}\{\chi(T_0<t)E_0(\exp[a\tau(t-T_0)]\chi(b_{t-T_0} \in \mathrm{d}x))\} \\ &\quad + E_{x_0}(\chi(T_0>t), b_t \in \mathrm{d}x) \\ &\equiv I_1 + I_2 \end{aligned} \tag{3.6}$$

where E_{x_0} is the conditional expectation of the path knowing that it starts at x_0 at $t=0$.

Suppose that $x_0>0$; it is well known that

$$\mathrm{Prob}_{x_0}(T_0 \in \mathrm{d}s) = (2\pi s^3)^{-1/2}x_0\exp(-x_0^2/2s)\,\mathrm{d}s$$

see [11, 12] so that in general

$$I_1 = \left(\int_0^t \mathrm{d}s(2\pi s^3)^{-1/2}|x_0|\exp(-x_0^2/2s)K(x, t-s\,|\,0)\right)\mathrm{d}x. \tag{3.7}$$

Moreover

$$I_2 = E_{x_0}(\chi(T_0 > t),\ b_t \in \mathrm{d}x)$$

is the solution of the Dirichlet problem

$$\partial u/\partial t = \tfrac{1}{2}\partial^2 u/\partial x^2 \qquad u(0, x) = \delta(x - x_0) \qquad u(t, 0) = 0$$

where x, x_0 are of the same sign and is 0 if x and x_0 are not of the same sign so

$$I_2 = (2\pi t)^{-1/2}[\exp(-|x_0 - x|^2/2t) - \exp(-|x_0 + x|^2/2t)] \qquad \chi(x, x_0 > 0)\,\mathrm{d}x. \tag{3.8}$$

Combining these results we obtain that the heat propagator of the potential $a\delta(x)$ is given by

$$K(x, t\,|\,x_0, 0) = [G_0(x - x_0, t) - G_0(x + x_0, t)]\chi(x_0 x > 0) + \int_0^{t_0} \mathrm{d}s(2\pi s^3)^{-1/2}|x_0| \exp(-x_0^2/2s)K(x, t - s\,|\,0) \tag{3.9}$$

where $G_0(x, t) = (2\pi t)^{-1/2}\exp(-x^2/2t)$ is the free Gaussian kernel. For example (3.9) can be simplified to

$$K(x, t\,|\,y, 0) = G_0(x - y, t) + a\int_0^{+\infty} \mathrm{d}u\ \mathrm{e}^{au}G_0(|x| + |y| + u, t). \tag{3.10}$$

We now check directly that this expression satisfies (3.3); it is clear that it satisfies the equation outside 0 with the appropriate initial condition.

At 0, the equation means that

$$\psi'(0^+) - \psi'(0^-) = -2a\psi(0).$$

We check this boundary condition directly:

$$\frac{\partial K}{\partial x}(0^+, t\,|\,y, 0) - \frac{\partial K}{\partial x}(0^-, t\,|\,y, 0) = 2a\int_0^{+\infty} \mathrm{d}u\ \mathrm{e}^{au}\frac{\partial}{\partial x}G_0(|x| + |y| + u, t)\Big|_{x=0} = 2a\int_0^{+\infty} \mathrm{d}u\left(\frac{\partial}{\partial u}(\mathrm{e}^{au}G_0) - G_0\frac{\partial \mathrm{e}^{au}}{\partial u}\right) \equiv -2aK(0, t\,|\,y, 0).$$

3.2. Using spectral resolution

We provide a second derivation of the propagator of equation (3.3). Consider the spectral resolution of

$$(\tfrac{1}{2}\partial^2/\partial x^2 + a\delta_0)u = -k^2 u. \tag{3.11}$$

This is satisfied by $\cos(\sqrt{2}k|x| - \delta(k))$, where the phase shift $\delta(k)$ is given by

$$\tan\delta(k) = -a/k\sqrt{2}. \tag{3.12}$$

Then

$$K(x, t\,|\,0) = C\int_{-\infty}^{+\infty} \exp(-k^2 t)\cos(\sqrt{2}k|x| - \delta(k))\cos\delta(k)\,\mathrm{d}k$$

assuming that the spectral function is a constant C. This last integral can be calculated and we obtain

$$\frac{1}{C} K(x, t|0) = \tfrac{1}{2} \int_{-\infty}^{+\infty} \exp(\mathrm{i}\sqrt{2}k|x|) \exp(-k^2 t)\, \mathrm{d}k$$
$$+ \tfrac{1}{2} \int_{-\infty}^{+\infty} \exp(-k^2 t) \exp[\mathrm{i}(\sqrt{2}k|x| - 2\delta(k))]\, \mathrm{d}k. \tag{3.13}$$

Using (3.12) and the identity

$$\frac{\mathrm{i}}{k - \mathrm{i}a\sqrt{2}} = \int_0^{+\infty} \exp[+\mathrm{i}\mu(k - \mathrm{i}a\sqrt{2})]\, \mathrm{d}\mu \qquad a < 0$$

we obtain

$$\int_{-\infty}^{+\infty} \exp(-k^2 t) \exp[\mathrm{i}(\sqrt{2}k|x| - 2\delta(k))]\, \mathrm{d}k$$
$$= \int_{-\infty}^{+\infty} \exp(-k^2 t) \exp(\mathrm{i}\sqrt{2}k|x|)\, \mathrm{d}k$$
$$+ \sqrt{2}a \int_0^{+\infty} \exp(\mu a\sqrt{2})\, \mathrm{d}\mu \int_{-\infty}^{+\infty} \exp(-k^2 t) \exp[\mathrm{i}(\sqrt{2}|x| + \mu)k]\, \mathrm{d}k. \tag{3.14}$$

On the right-hand side we see that the free propagator appears. Adjusting C so that for $t \to 0^+$ $K(x, t|0) \to \delta(x)$, we obtain the same formula as (3.10) for $y = 0$.

3.3. *A periodic propagator*

We use the preceding method to obtain an explicit example of a propagator in a periodic potential.

We consider the unit circle parametrised by $x \in [-\pi, \pi]$ with periodic boundary conditions and consider the Schrödinger equation

$$\{\partial^2/\partial x^2 + a[\delta(x) - \delta(x - \pi)]\}u = -k^2 u \tag{3.15}$$

with 2π periodic condition on u.

We define the Jacobi theta function

$$\theta_3(z, t) = \sum_{k=-\infty}^{+\infty} \exp(\mathrm{i}\pi t k^2) \exp(2k\mathrm{i}z). \tag{3.16}$$

As before, the δ potential is expressed as a boundary condition. Using $\theta_3(x) \to 2\pi\delta(x)$ if $t \to 0$, we find as above that

$$K(x, t|0) = \frac{1}{2\pi} \theta_3\left(\frac{|x|}{2}, \frac{\mathrm{i}t}{2\pi}\right) + \frac{a}{2\pi} \int_0^{+\infty} \mathrm{e}^{\mu a} \theta_3\left(\frac{|x| + \mu}{2}, \frac{\mathrm{i}t}{2\pi}\right) \mathrm{d}\mu. \tag{3.17}$$

This is formally similar to the non-periodic case (3.10) except that we replace G_0 by a Jacobi theta function. The general case $K(x, t|y, 0)$ follows from (3.10) by replacing G_0 by the Jacobi theta function.

3.4. Physical time in the Schrödinger equation and semiclassical approximation

For the physical time in the Schrödinger equation, the 'time' of our heat kernel formulae becomes pure imaginary. We denote the Schrödinger propagator by $G(x, t|y)$ so that $(H - \mathrm{i}\partial/\partial t)\, G = 0$ and G is obtained from the K of (3.10) by the replacement $t \to \mathrm{i}t$. In particular for the free particle

$$G_0(x, t|y) = (2\mathrm{i}\pi t)^{-1/2} \exp[\mathrm{i}(x-y)^2/2t] \tag{3.18}$$

and for $H = -\frac{1}{2}\partial^2/\partial u^2 - a\delta(x)$

$$G(x, t|y) = G_0(x, t|y) + a \int_0^{+\infty} \mathrm{d}u\, \mathrm{e}^{au} G_0(|x|+|y|+u, t|0). \tag{3.19}$$

Until now, we have written $\hbar = 1$ to simplify the notation. First we reinstall $\hbar$ in the time-dependent propagator (3.19) to yield

$$G(x, t|y) = (2\pi\hbar \mathrm{i} t)^{-1/2} \exp[\mathrm{i}(x-y)^2/2\hbar t] + \frac{a}{\hbar^2} \int_0^{+\infty} \mathrm{d}u (2\mathrm{i}\pi\hbar t)^{-1/2} \exp\left(\frac{au}{\hbar^2} + \frac{\mathrm{i}(\xi+u)^2}{2\hbar t}\right) \tag{3.20}$$

where $\xi = |x| + |y|$. In principle the semiclassical approximation for G would be the replacement of G by $\exp(\mathrm{i}S(x, t; y)/\hbar)$ with S the classical action. However, this is not particularly informative for the following reasons.

First consider the case $a < 0$ (i.e. repulsive δ function). In the spirit of (3.1), this can be thought of as the limit of repulsive step functions of width ε, height $-a/\varepsilon$ (ε tends to 0).

For $y < 0$ and $x > 0$ and given t, there is in fact a classical path for any positive non-zero ε, but a simple calculation shows that the classical action along this path is asymptotic to $\frac{1}{2}(x-y)(-2a/\varepsilon)^{1/2}$ and this tends to ∞ for $\varepsilon \to 0$. To the extent that meaningful conclusions can be drawn from this, it suggests there should be no transmission through the barrier in the $\hbar \to 0$ limit (imagine ε held fixed at a small value; then the large value of $S \sim 1/\sqrt{\varepsilon}$ will make the integral using $\exp(\mathrm{i}S/\hbar)$ have rapidly varying phase beyond that already due to $1/\hbar$).

In fact, this preliminary conclusion is not entirely misleading since we can examine the small $\hbar$ approximation for G in (3.19).

For the case of interest $x > 0 > y$, ξ also equals $x - y$. For the integral over u, we do an asymptotic expansion which, because there are no stationary points on the contour of integration, is given simply by the terms in the exponential linear in u; thus

$$G(x, t|y) \sim (2\mathrm{i}\pi\hbar t)^{-1/2} \exp(\mathrm{i}\xi^2/2\hbar t)\left[1 + \frac{a}{\hbar^2}\int_0^{+\infty} \mathrm{d}u \exp\left(\frac{au}{\hbar^2} + \frac{\mathrm{i}\xi u}{\hbar t}\right)\right]. \tag{3.21}$$

Recall $a < 0$; we perform the integral; its leading term precisely cancels that from G_0 so that

$$G(x, t|y) \sim \frac{\mathrm{i}\xi\hbar}{at} \frac{\exp(\mathrm{i}\xi^2/2\hbar t)}{(2\mathrm{i}\pi\hbar t)^{1/2}}. \tag{3.22}$$

This is smaller by a factor $\hbar$ than the usual propagator, giving more precise information than the hints obtained from an earlier semiclassical calculation. For the case that x and y have the same sign, there is no exact cancellation since now $\xi = |x| + |y| \neq x - y$ and a short calculation shows that the δ function now acts like a mirror with an order $\hbar$ term getting through the mirror.

The failure of the semiclassical approximation in this case can be ameliorated by redefining that approximation in the manner of Keller's geometric diffraction theory. That is, to lowest order, paths do not get through the δ function, but there is a 'diffracted ray propagator', reduced by a factor $\hbar$ which is given by (3.22). Its strength is also, reasonably, inversely proportional to $|a|$. This is in the spirit of Keller's work [13] where an exact solution was used to suggest the form of diffracted rays that entered regions inaccessible in classical geometrical optics.

Now, consider the case $a>0$ (an attractive δ function). Again a simple classical mechanics calculation gives $S \sim (\xi^2/2t)(\xi = x-y, x>0>y)$ with only $O(\sqrt{\varepsilon})$ corrections due to the well of depth a/ε and width ε. The $\hbar \to 0$ limit of (3.20) is trickier since the integral ostensibly diverges in the sense of functions, but it is standard procedure to assume a small imaginary part in the mass (not explicitly written in our formulae) to ensure convergence. The growing exponential in (3.20) now implies that the integral will be of maximum norm for large positive u, so that we extend the integral to $-\infty$ and integrate formally. More precisely we write

$$\frac{a}{\hbar^2}\int_0^{+\infty} \mathrm{d}u \exp\left(\frac{au}{\hbar^2}+\frac{\mathrm{i}(\xi+u)^2}{2\hbar t}\right)$$

$$=\frac{a}{\hbar^2}\int_{-\infty}^{+\infty}-\frac{a}{\hbar^2}\int_{-\infty}^{0}$$

$$=\frac{a}{\hbar^2}\int_{-\infty}^{+\infty}-\frac{a}{\hbar^2}\int_{0}^{+\infty} \mathrm{d}v \exp\left(-\frac{av}{\hbar^2}+\frac{\mathrm{i}(\xi-v)^2}{2\hbar t}\right).$$

However, this last integral is exactly the one which was computed in (3.21) (except for a change $a \to -a$, $\xi \to -\xi$) and so it exactly cancels the G_0 term which is insensitive to a and to the sign of ξ and leaves a term of the form (3.22). Therefore

$$G(x,t\,|\,y) \sim \frac{\mathrm{i}\xi\hbar}{at} G_0(\xi, t\,|\,0)+\frac{\exp(-a\xi/\hbar^2)}{(2\pi\mathrm{i}\hbar t)^{1/2}}\frac{a}{\hbar^2}\int_{-\infty}^{\infty}\mathrm{d}v \exp(\mathrm{i}v^2/2\hbar t+av/\hbar^2)$$

$$=\frac{\mathrm{i}\xi\hbar}{at} G_0(\xi, t\,|\,0)+\frac{a}{\hbar^2}\exp(-a\xi/\hbar^2)\exp(\mathrm{i}a^2t/2\hbar^3). \tag{3.23}$$

Although the second term in this expression appears large for $\hbar \to 0$ it is in fact the ground state contribution to the time-dependent Green function and is significant only in the small region $|x|+|y| \leq \hbar^2/a$. This result is totally at variance with the semiclassical hint which suggested that the attractive δ function should be invisible. In fact it is as fully effective as a barrier as the repulsive potential except for a small enhancement near the origin.

4. Combination of a potential and a δ function

Let $H_V = -\frac{1}{2}\mathrm{d}^2/\mathrm{d}x^2 + V(x)$

$$H_1 = \lambda W(x).$$

Call $G_V(x, t\,|\,y)$ the propagator for

$$\mathrm{i}\,\partial/\partial t = H_V$$

and K the propagator for

$$\mathrm{i}\,\partial/\partial t = H_V + H_1.$$

We obviously have the integral equation

$$K(x,t|y) = G_V(x,t|y) - \mathrm{i}\int_0^t \mathrm{d}s \int \mathrm{d}z\, G_V(x,s|z)W(z)K(z,t-s|y).$$

For $W(z) = \lambda\delta(z)$, this equation becomes

$$K(x,t|y) = G_V(x,t|y) - \mathrm{i}\lambda \int_0^t \mathrm{d}s\, G_V(x,s|0)K(0,t-s|y). \tag{4.1}$$

We call

$$\varphi_V(s) = G_V(0,s|0) \qquad \varphi(s) = K(0,s|0)$$

and

$$\hat{\varphi}_V(\mu) = \int_0^{+\infty} \mathrm{e}^{-\mu t}\varphi_V(s)\,\mathrm{d}s$$

and the same for $\varphi(s)$. Then the Laplace transform of (4.1) gives

$$\hat{\varphi}(\mu) = \hat{\varphi}_V(\mu)/(1+\mathrm{i}\lambda\hat{\varphi}_V(\mu)). \tag{4.2}$$

If we can explicitly invert the Laplace transform of (4.2) we immediately obtain

$$K(x,t|0) = G_V(x,t|0) - \mathrm{i}\lambda \int_0^t \mathrm{d}s\, G_V(x,s|0)\varphi(t-s)$$

and then by (4.1) the general kernel $K(x,t|y)$.

The advantage of this method is that we do not have to compute (or guess) the proper spectral function.

4.1. The propagator for a periodic Dirac potential

We consider the following potential:

$$W(x) = a\sum_{n=-\infty}^{+\infty} \delta(x-nL) \tag{4.3}$$

and we want to find the propagator for the heat equation

$$\partial/\partial t = \tfrac{1}{2}\partial^2\partial x^2 + W(x). \tag{4.4}$$

As usual, we call G_0 the free propagator

$$G_0(x,t|y) = \frac{1}{(2\pi t)^{1/2}}\exp\left(-\frac{|x-y|^2}{2t}\right).$$

If $G(x,t|y)$ is the propagator with the periodic Dirac potential, we have by integrating (4.4)

$$G(x,t|y) = G_0(x,t|y) + \sum_n a\int_0^t \mathrm{d}s\, G_0(x,t-s|nL)G(nL,s|y). \tag{4.5}$$

Define

$$\hat{f}(\mu)=\int_0^{+\infty} e^{-\mu t}f(t)\,dt$$

for any function $f(t)$. We have in particular

$$\hat{G}_0(x,\mu\,|\,y)=\frac{1}{(2\mu)^{1/2}}\exp(-\sqrt{2\mu}|x-y|). \tag{4.6}$$

Take $y=0$, $x=jL$ (j integer) in (3.5) and take the Laplace transform of (4.5). Taking into account (4.6), we obtain

$$\hat{G}(jL,\mu\,|\,0)=\frac{1}{(2\mu)^{1/2}}\exp(-\sqrt{2\mu}|j|L)+\sum_n a\frac{1}{(2\mu)^{1/2}}\exp(-\sqrt{2\mu}|j-n|L)\hat{G}(nL,\mu\,|\,0).$$

This can be rewritten as an infinite system of linear equations for the unknown numbers

$$X_j=\hat{G}(jL,\mu\,|\,0) \tag{4.7}$$

with the given Y_j

$$Y_j=\frac{\exp[-(2\mu)^{1/2}|j|L]}{(2\mu)^{1/2}}$$

$$\sum_{n=-\infty}^{+\infty}[\delta(j-n)-aY_{j-n}]X_n=Y_j.$$

Define

$$\hat{X}(\theta)=\sum_{j=-\infty}^{+\infty}e^{ij\theta}X_j$$

$$\hat{Y}(\theta)=\sum_{j=-\infty}^{+\infty}e^{ij\theta}Y_j=\frac{1}{(2\mu)^{1/2}}\frac{1-\exp[-2(2\mu)^{1/2}L]}{|1-e^{i\theta}\exp[-(2\mu)^{1/2}L]|^2}.$$

We deduce immediately that for any θ

$$(1-a\hat{Y}(\theta))\hat{X}(\theta)=\hat{Y}(\theta)$$

and

$$X_j=\frac{1}{2\pi}\int_0^{2\pi}e^{-ij\theta}\hat{X}(\theta)\,d\theta=\frac{1}{2\pi}\int_0^{2\pi}e^{-ij\theta}\frac{\hat{Y}(\theta)}{1-a\hat{Y}(\theta)}\,d\theta.$$

We can also take $j\geqslant 0$; a trivial computation gives

$$\frac{\hat{Y}(\theta)}{1-a\hat{Y}(\theta)}=\frac{A}{1-2\xi\cos\theta}$$

where

$$A=\frac{1-\exp[-2(2\mu^{1/2}L]}{(2\mu)^{1/2}(1+\exp[-2(2\mu)^{1/2}L]-a\{1-\exp[-2(2\mu)^{1/2}L]\})}$$

$$\xi=\frac{\exp[-2(2\mu)^{1/2}L]}{1+\exp[-2(2\mu)^{1/2}L]-a\{1-\exp[-2(2\mu)^{1/2}L]\}} \tag{4.8}$$

and so at least for a sufficiently small

$$\frac{\hat{Y}(\theta)}{1-a\hat{Y}(\theta)}=A\sum_{n\geq 0}\xi^n 2^n\cos^n\theta.$$

However

$$\frac{1}{2\pi}\int_0^{2\pi}\mathrm{e}^{-\mathrm{i}j\theta}2^n\cos^n\theta\,\mathrm{d}\theta=\sum_{n=0}^{n}\binom{n}{k}\delta(2k-j-n)$$

and we have to consider two cases.

(1) j is even; $j=2\bar{j}$.

Then n must be even; $n=2q$ and

$$X_{2\bar{j}}=A\sum_{q\geq\bar{j}}\xi^{2q}\binom{2q}{q+\bar{j}}=A\xi^{2\bar{j}}\sum_{q\geq 0}\frac{\xi^{2q}}{q!}\frac{(2q+2\bar{j})!}{(2\bar{j}+q)!}$$

and so

$$X_{2\bar{j}}=A\xi^{2\bar{j}}F(\bar{j}+\tfrac{1}{2},\bar{j}+1;2\bar{j}+1;(2\xi)^2)$$

where $F(\alpha,\beta;\gamma;z)$ denotes the hypergeometric function.

(2) j is odd; $j=2\bar{j}+1$.

Then n must be odd; $n=2q-1$ and

$$X_{2\bar{j}+1}=A\sum_{q=\bar{j}+1}^{+\infty}\xi^{2q-1}\binom{2q-1}{q+\bar{j}}-A\xi^{2\bar{j}+1}\sum_{q=0}^{+\infty}\frac{\xi^{2q}}{q!}\frac{(2\bar{j}+1+2q)!}{(2\bar{j}+1+q)!}$$

and so

$$X_{2\bar{j}+1}=A\xi^{2\bar{j}+1}F(\bar{j}+\tfrac{3}{2},\bar{j}+1;2\bar{j}+2;(2\xi)^2).$$

In both cases, this can be rewritten as

$$X_j=A\xi^jF(\tfrac{1}{2}j+1,\tfrac{1}{2}j+\tfrac{1}{2};j+1;(2\xi)^2).$$

If we recall that X_j was defined by (4.7) and A and ξ by (4.8), we can rewrite this as

$$\hat{G}(jL,\mu\,|\,0)=A\xi^jF(\tfrac{1}{2}j+1,\tfrac{1}{2}j+\tfrac{1}{2};j+1;(2\xi)^2)\tag{4.9}$$

with j a positive integer and

$$A=\frac{1-\exp[-2(2\mu)^{1/2}L]}{\sqrt{2\mu}(1+\exp[-2(2\mu)^{1/2}L]-a\{1-\exp[-2(2\mu)^{1/2}L]\})}$$

$$\xi=\frac{\exp[-2(2\mu)^{1/2}L]}{1+\exp[-2(2\mu)^{1/2}L]-a\{1-\exp[-2(2\mu)^{1/2}L]\}}$$

and we can recover the time-dependent propagator by simply inverting the Laplace transform (recall that μ is the Laplace variable associated with t). Clearly the general propagator between two general points is much more complicated.

4.2. A Dirac potential in a square well

We consider now an infinite square well of length $2b$ and centre 0. The associated potential is then

$$V(x)=\begin{cases}0 & \text{if } |x|<b\\ \infty & \text{if } |x|>b.\end{cases}$$

We call H_0 the Hamiltonian of this square well; H_0 is just $-\frac{1}{2}\,\mathrm{d}^2/\mathrm{d}x^2$ with boundary conditions 0 at $\pm b$. The propagator of the square well denoted by $G_{\mathrm{SW}}(x, t\,|\,y)$ is defined by the formula

$$G_{\mathrm{SW}}(x, t\,|\,y) = \sum_{n=-\infty}^{+\infty} [G_0(x-y+4nb, t\,|\,0) - G_0(x+y+2b(2n+1), t\,|\,0)]$$

for $|x|$ and $|y| < b$

$$G_{\mathrm{SW}}(x, t\,|\,y) = 0 \qquad \text{if } |x| \text{ or } |y| > b \tag{4.10}$$

and $G_0(x, t\,|\,y)$ is the usual free space propagator. In fact, it is clear that $G_{\mathrm{SW}}(x, t\,|\,y)$ satisfies the propagation equation in $|x| < b$ and tends to $\delta(x-y)$ if $t \to 0^+$. Moreover, it satisfies the boundary condition

$$G_{\mathrm{SW}}(\pm b, t\,|\,y) = 0$$

because if we take the term $G_0(b-y+4nb, t\,|\,0)$ in (4.15) it has an exponent containing $|y-(4n+1)b)|^2$ and this exactly cancels the term $-G_0(b+y+2b(2p+1), t\,|\,0)$ which has an exponent containing $|y+(4p+2+1)b|^2$ if $4p+2+1 = -(4n+1)$ or $p = -n-1$.

Let us now put a Dirac potential of intensity $-a$ at point 0. The Hamiltonian is then $H = -\frac{1}{2}\,\mathrm{d}^2/\mathrm{d}x^2 - a\delta(x)$ on $[-b, +b]$ with boundary conditions 0 at $\pm b$. The propagator for this Hamiltonian H is $G(x, t\,|\,y)$ defined by the formula

$$G(x, t\,|\,y) = G_{\mathrm{SW}}(x, t\,|\,y) + a\int_0^{+\infty} \mathrm{d}u\; \mathrm{e}^{au} G_{\mathrm{SW}}(|x|+|y|+u, t\,|\,0) \tag{4.11}$$

(with the convention (4.10) if $|x|+|y|+u > b$).

In fact, it is clear that $G(x, t\,|\,y)$ satisfies the propagation equation outside 0 in $[-b, +b]$ and also the boundary condition at $\pm b$. The only problem is to check the boundary condition at 0. Fix $y \neq 0$ in $[+b, +b]$

$$G(x, t\,|\,y) = G_{\mathrm{SW}}(x, t\,|\,y) + a\int_0^{b-|x|-|y|} \mathrm{d}u\; \mathrm{e}^{au}\, G_{\mathrm{SW}}(|x|+|y|+u, t\,|\,0)$$

and so

$$\frac{\partial G}{\partial x}(0^+, t\,|\,y) - \frac{\partial G}{\partial x}(0^-, t\,|\,y) = 2a\int_0^{b-|y|} \mathrm{d}u\; \mathrm{e}^{au}\frac{\partial G_{\mathrm{SW}}}{\partial x}(|y|+u, t\,|\,0).$$

(we have used the boundary condition at b).

Integrating by parts and remarking that

$$G_{\mathrm{SW}}(|y|, t\,|\,0) = G_{\mathrm{SW}}(y, t\,|\,0) = G_{\mathrm{SW}}(0, t\,|\,y)$$

we obtain the boundary condition at 0

$$\frac{\partial G}{\partial x}(0^+, t\,|\,y) - \frac{\partial G}{\partial x}(0^-, t\,|\,y) = 2aG(0, t\,|\,y).$$

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