TOTAL ABSORPTION IN FINITE TIME IN AN \( i\delta \) POTENTIAL

by

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ABSTRACT

We consider the evolution of Green’s function of the one-dimensional Schrödinger equation in the presence of the complex potential \(-ik\delta(x)\). Our result is the construction of an explicit time-dependent solution which we use to calculate the time-dependent survival probability of a quantum particle. The survival probability decays to zero in finite time, which means that the complex delta potential well is a total absorber for quantum particles. This potential can be interpreted as a killing measure with infinite killing rate concentrated at the origin.

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The fundamental question of the existence of a totally absorbing potential that absorbs a particle in finite time with probability 1 has been the subject of extensive discussion in the literature [1], [2]. It was claimed that no perfectly absorbing potential can exist. To study this question, we consider the model experiment of releasing electrons at an absorbing plane placed at the origin. This model has many uses, e.g., in scattering theory, solid state physics, surface dynamics, physical chemistry and so on [3]-[5]. The problem can be described [5] by the one-dimensional Schrödinger equation with the complex potential \(-ik\delta(x), (k > 0)\). The description proposed in [5] considers a time-independent monochromatic wave at \(-\infty\) that is measured at \(+\infty\) (on the other side of the absorbing plane). This is the standard time-independent description of scattering of plane waves on an absorbing plane. The result of [5] is that up to 25% of the incident current is absorbed by the plane.

A related time-independent description of this problem is due to Muga et al. [4], [6]. In this description a complex potential of finite, though arbitrarily small support, absorbs totally any discrete set of plane waves. This precludes the possibility of absorbing a normalizable wave packet.

In our time-dependent description of the same experiment electrons are released at the absorbing plane one at a time. Their survival probability, \(S(t)\), is defined as the relative number of electrons that have not been absorbed by the surface by time \(t\) since their release. We show that in this description there is a critical time beyond which the survival probability of an electron vanishes. This means that the given potential leads to an eventual total absorption of all electrons released in finite time with probability 1. This is in contrast to the assertion of the time-independent model of this experiment. We also show that the probability density on the surface converges in time to a finite limit, though the total probability in space decays in time.

This description of an absorbing surface is different from the one proposed in [7] and [8]. The description in [7], [8] assumes that the surface absorbs all Feynman trajectories at the moment they reach the absorbing surface. The difference in the results of the two time-dependent descriptions is that in the present description the wave function can propagate across the surface while in the description proposed in [7] and [8] it cannot. While the result of [7], [8] is that the survival probability decays at and exponential rate proportional to the absorption current at the absorbing plane, the result of the present description is that the survival probability decays in finite time.

**Free Brownian motion with \(\delta\)-killing**

Consider the Brownian motion on the line with a killing measure \(k\delta(x)\) per unit time. The transition probability density satisfies the diffusion equation

\[
p_t = Dp_{xx} - \kappa\delta(x)p,
\]

or equivalently,

\[
p_t(x,t) = Dp_{xx}(x,t) - \kappa \delta(x)p(0,t),
\]
and the initial condition

\[ p(x,0) = \delta(x - x_0). \]  

(2)

The survival probability is given by

\[ S(t) = \int p(x,t) \, dx, \]

The diffusion equation gives

\[ \frac{d}{dt} \int p(x,t) \, dx = -\kappa p(0,t), \]

hence

\[ S(t) = 1 - \kappa \int_0^t p(0,t) \, dt. \]

Changing variables to \( Dt = \tau \), the solution of the initial value problem (1), (2) satisfies

\[ p(x,\tau) = \int_{-\infty}^{\infty} \frac{1}{2\sqrt{\pi \tau}} \exp \left\{ -\frac{(x - y)^2}{4\tau} \right\} \delta(y - x_0) \, dy - \int_0^\tau \frac{1}{2\sqrt{\pi (\tau - \sigma)}} \int_{-\infty}^{\infty} \exp \left\{ -\frac{(x - y)^2}{4(\tau - \sigma)} \right\} \frac{\kappa}{D} \delta(y) p(y,\sigma) \, dy \, d\sigma, \]

and in particular it satisfies the integral equation

\[ p(0,\tau) = \frac{1}{2\sqrt{\pi \tau}} \exp \left\{ -\frac{x_0^2}{4\tau} \right\} - \int_0^\tau \frac{1}{2\sqrt{\pi (\tau - \sigma)}} \frac{\kappa}{D} p(0,\sigma) \, d\sigma. \]  

(3)

The Laplace transform of the integral equation (3) is

\[ \hat{p}(0,s) = \frac{e^{-x_0\sqrt{s}}}{2\sqrt{s}} - \frac{\kappa \hat{p}(0,s)}{2D\sqrt{s}}, \]

hence [9, p.1026, eq.(29.3.88)],

\[ p(0,\tau) = \frac{1}{2} \mathcal{L}^{-1} \left( \frac{e^{-x_0\sqrt{s}}}{\sqrt{s} + \frac{\kappa}{2D}} \right) \]

\[ = \frac{1}{2} \left\{ \frac{1}{\sqrt{\pi \tau}} \exp \left\{ -\frac{x_0^2}{4\tau} \right\} - \frac{\kappa}{2D} e^{\frac{x_0^2}{4D\tau}} e^{\frac{\kappa^2}{4D\tau}} \left[ 1 - \text{erf} \left( \frac{\kappa \sqrt{\tau} + x_0}{2\sqrt{\tau}} \right) \right] \right\} \]

\[ \sim \frac{1}{2} \frac{\kappa x_0 + 2D \sqrt{\pi} D}{\kappa^2 \tau^{3/2}} \quad \text{for} \quad \tau \to \infty. \]  

(4)
It follows that the large $\tau$ limit of $p(0, \tau)$ is
\[
\lim_{s \to 0} \frac{se^{-x_0\sqrt{s}}}{2\sqrt{s} + \frac{\kappa}{D}} = 0.
\]
The limit of the integral of $\frac{\kappa}{D}p(0, \tau)$ is
\[
\lim_{\tau \to \infty} \frac{\kappa}{D} \int_{0}^{\tau} p(0, u) \, du = \lim_{s \to 0} \frac{\kappa}{D} \hat{p}(0, s) = \lim_{s \to 0} \frac{\kappa}{D} e^{-x_0\sqrt{s}} = 1.
\]
It follows that the survival probability decays to zero.

The survival probability decays as
\[
\frac{\kappa}{D} \int_{\tau}^{\infty} p(0, \tau) \, d\tau = \frac{x_0 + 2D/\kappa}{\sqrt{\pi \tau}} + O\left(\frac{1}{\tau^{3/2}}\right) \quad \text{for} \quad \tau \gg 1.
\]

**The survival probability in Schrödinger’s equation with $-ik\delta$ potential**

The wave function in the presence of the potential $-ik\delta(x)$ can be expressed as the Feynman integral with killing rate $k\delta(x)$ \([10]\). This means that at each time step in the construction of the Feynman integral the wave amplitude is discounted by the factor $1 - \frac{1}{2}k\delta(x(t)) \Delta t$. The $\delta$-function can be interpreted as the usual limit of high and narrow rectangular potential whose area is 1. We recall that the limit of a high rectangular potential with finite width leads to total reflection rather than total absorption. This discount factor corresponds to the additional factor
\[
\exp\left\{ -\frac{k}{2} \delta(x) \Delta t \right\}
\]
in the propagator. The resulting Schrödinger equation contains the imaginary potential $-\frac{ik}{2} \delta(x)$,
\[
\hbar \psi_t = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi - \frac{ik}{2} \delta(x)\psi. \quad (6)
\]
We assume for simplicity that
\[
\psi(y, 0) = \delta(y - x_0) \quad (7)
\]

When the initial condition is square-integrable, we obtain from (6) that
\[
\frac{d}{dt} \int |\psi(x, t)|^2 \, dx = -\frac{k}{\hbar} |\psi(0, t)|^2,
\]
so that the survival probability is given by

$$S(t) = \int |\psi(x,t)|^2 dx = 1 - k \int_0^t |\psi(0,t)|^2 dt. \quad (8)$$

To evaluate $S(t)$, we have to determine the decay rate of $\psi(0,t)$. To do so, we begin with Green’s function of the Schrödinger equation

$$i\hbar G_t = -\frac{\hbar^2}{2m} \Delta_x G + V(x)G$$

and the initial condition

$$\lim_{t \to 0} G(x, y, t) = \delta(x - y).$$

In the case of free propagation

$$G(x, y, t) = \sqrt{\frac{m}{2\pi\hbar}} \exp\left\{-\frac{m(x - y)^2}{2\hbar}\right\}. \quad (9)$$

The solution of (8) can be written as

$$\psi(x, t) = \int G(x, y, t)\psi(y, 0) dy - \frac{i\hbar}{2} \int_0^t \int G(x, y, t - s)\delta(y)\psi(y, s) dy ds$$

$$= \int G(x, y, t)\psi(y, 0) dy - \frac{i\hbar}{2} \int_0^t G(x, 0, t - s)\psi(0, s) ds. \quad (10)$$

With the initial condition (7), we obtain

$$\psi(0, t) = \int G(0, y, t)\psi(y, 0) dy - \frac{i\hbar}{2} \int_0^t G(0, 0, t - s)\psi(0, s) ds. \quad (11)$$

Equation (11) is an integral equation for the function $\phi(t) = \psi(0, t)$, that can be written as

$$\phi(t) = f(t) - \int_0^t K(t - s)\phi(s) ds, \quad (12)$$

where

$$f(t) = G(0, x_0, t) = \sqrt{\frac{m}{2\pi\hbar}} \exp\left\{-\frac{mx_0^2}{2\hbar}\right\}$$

$$K(t) = \frac{i\hbar}{2} G(0, 0, t) = k \sqrt{\frac{im}{2\pi\hbar}}. \quad (13)$$

The Laplace transform of the solution of eq.(13) is given by

$$\hat{\phi}(s) = \frac{\hat{f}(s)}{1 + K(s)}.$$
where

\[ \hat{f}(s) = \sqrt{\frac{m}{2\hbar s}} \int e^{-\sqrt{\frac{2m\alpha^2}{\hbar^2}}} \psi(y, 0) \, dy \]

and

\[ \hat{K}(s) = \frac{k}{2} \sqrt{\frac{im}{2\hbar s}}. \]

The exact expression for \( \phi(t) \) is obtained from eq.(14) with the values

\[ \tau = Dt, \quad D = \frac{i\hbar}{2m}, \quad \kappa = \frac{k}{2\hbar}. \]

It is given by

\[ \phi(t) = \frac{\sqrt{m}}{\sqrt{2\pi\hbar t}} \int_{-\infty}^{\infty} e^{\frac{i}{2\hbar^2}m^2} \psi(y, 0) \, dy + \] \[ \frac{1}{4} \frac{i}{\hbar^2} m e^{-\frac{1}{2} \frac{i}{\hbar^2} m^2 t} \int_{-\infty}^{\infty} e^{-\frac{1}{2} \frac{i}{\hbar^2} m^2 y} \times \] \[ \left[ 1 - \text{erf} \left( -\frac{1}{4} \frac{k}{\hbar} \sqrt{2 \left( \frac{i\hbar t}{m} \right)} + \frac{1}{2} y \frac{\sqrt{2}}{\left( \frac{i\hbar t}{m} \right)} \right) \right] \psi(y, 0) \, dy. \]

Choosing

\[ \psi(y, 0) = \frac{1}{\sqrt{2\pi a}} \exp \left( -\frac{(y - x_0)^2}{2a^2} \right), \]

the first integral is

\[ (1 - i) \frac{\sqrt{m}}{2\sqrt{(-ima^2 + \hbar t)\sqrt{\pi}}} \exp \left( \frac{1}{2} \frac{i}{a^2} - \frac{m}{ima^2 + \hbar t} \right). \]

To evaluate the second integral, we note that at the point \( y = -\frac{1}{2} \frac{k}{\hbar} \left( 1 - \frac{1}{\sqrt{t}} \right) \) the argument of the error function vanishes, so it cannot be expanded uniformly for large \( t \). Therefore, we break the line into the segments \(-\infty < y < -\frac{1}{2} \frac{k}{\hbar} \left( 1 - \frac{1}{\sqrt{t}} \right) + \alpha \sqrt{t}, \) and \(-\frac{1}{2} \frac{k}{\hbar} \left( 1 - \frac{1}{\sqrt{t}} \right) + \alpha \sqrt{t} < y < \infty, \) where \( \alpha \) is a positive constant to be chosen. The integral over the first interval can be estimated by

\[ \int_{-\infty}^{-\frac{1}{2} \frac{k}{\hbar} \left( 1 - \frac{1}{\sqrt{t}} \right) + \alpha \sqrt{t}} \exp \left( -\frac{(y - x_0)^2}{2a^2} \right) \, dy \sim \] \[ \exp \left\{ -\left( \frac{1}{2} \frac{k}{\hbar} \left( 1 - \frac{1}{\sqrt{t}} \right) - \alpha \sqrt{t} - x_0 \right)^2 \frac{2a^2}{2a^2} \right\} \to 0 \quad \text{as} \quad t \to \infty \]
and the convergence rate is exponential in $t^2$. In the second interval the error function can be expanded asymptotically for large $t$ as [1]

$$
\frac{1}{4} \frac{k}{\hbar^2} me^{-\frac{1}{2} \frac{k^2}{m} t^2} \int_{-\infty}^{\infty} e^{-\frac{i k}{\hbar} \left(1 - \frac{1}{\sqrt{m}} y^2 \right)} \times \left[1 - \text{erf} \left(-\frac{1}{4} \frac{k}{\hbar^2} m \sqrt{2} \sqrt{(\hbar \frac{m}{2})} + \frac{1}{2} y \sqrt{\left(\hbar \frac{m}{2}\right)} \right) \right] \psi(y, 0) \, dy
$$

Expanding each term in the sum in powers of $y$ and using Watson’s lemma, we find that higher powers in $y$ produce lower powers of $t$ in the large $t$ asymptotic expansion of the integral. It follows that the leading order term in the large $t$ expansion comes from the first term 1. Since $ikt + y \neq 0$, we can evaluate the first term by extending the interval of integration over the entire line with an error that decays exponentially fast in $t^2$. In particular, setting $y = 0$, we obtain the leading order contribution as

$$
\frac{1}{4} \frac{k}{\hbar^2} me^{-\frac{1}{2} \frac{k^2}{m} t^2} \int_{-\infty}^{\infty} e^{-\frac{i k}{\hbar} \left(1 - \frac{1}{\sqrt{m}} y^2 \right)} \times \left\{-\frac{k \sqrt{h \hbar} t}{\sqrt{2 \pi m} (ikt + y)} \left(1 - \sum_{n=1}^{\infty} (-1)^n \frac{\Pi_{j=1}^n (2j - 1)}{\left(2 \left(\frac{1}{2} \sqrt{\frac{h \hbar}{2m}} + y \sqrt{\frac{m}{2h \hbar}}\right)^2\right)^n}\right)\right\} \psi(y, 0) \, dy
$$

$$
\sim -\frac{1}{16} \frac{i \sqrt{(-1)}}{h} \sqrt{(ima^2 + h t)} \frac{\sqrt{m}}{\sqrt{\pi}} \exp \left(\frac{1}{8} i m \frac{4x_0^2 h^3 + ik^2 tma^2 - k^2 t^2 h}{(-ima^2 + h t) h^3}\right)
$$

It follows that

$$
\phi(t) \sim (1 - i) \frac{\sqrt{m}}{2\sqrt{(-ima^2 + h t)\sqrt{\pi}}} \exp \left(\frac{1}{2} i x_0^2 \frac{m}{-ima^2 + h t}\right) -
\frac{1}{16} \frac{i \sqrt{(-1)}}{h} \sqrt{(ima^2 + h t)} \frac{\sqrt{m}}{\sqrt{\pi}} \exp \left(\frac{1}{8} i m \frac{4x_0^2 h^3 + ik^2 tma^2 - k^2 t^2 h}{(-ima^2 + h t) h^3}\right)
$$
Since the first term is not oscillatory for large $t$ and the second term is oscillatory, we find that

$$|\phi(t)|^2 = O\left( t^{-1} \right)$$

for large $t$.

It follows that the large $t$ asymptotics of $S(t)$ is

$$S(t) \sim 1 - O(\ln t).$$

Higher order terms in the asymptotic expansion of $\phi(t)$ contribute integrable terms to $S(t)$. Thus $S(t)$ vanishes in finite time.

This means that the wave function vanishes in finite time everywhere outside $x = 0$. That is, it develops a discontinuity in finite time. From that time on, the expression eq.(10), with $\psi(0, t) = \phi(t)$ given by eq.(14), is no longer a solution of Schrödinger’s equation. After this time $\psi(x, t)$ vanishes identically outside $x = 0$.

We conclude that the potential $-ik\delta(x)$ leads to total absorption of the wave function in finite time.

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