An Exact Solution to the Time-dependent Schrödinger Equation for a Model One-dimensional Potential

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Abstract

Analytical solutions to the time-dependent Schrödinger equation in one dimension are developed for time-independent potentials, one consisting of an infinite wall and a repulsive delta function. An exact solution is obtained by means of a convolution of time-independent solutions spanning the given Hilbert space with appropriately chosen spectral functions. Square-integrability and the boundary conditions are satisfied. The probability for the particle to be found inside the potential well is calculated and shown to exhibit non-exponential decay decreasing at large times as $t^{-3}$. The result is generalized for all square-integrable solutions to this problem.

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1 Introduction

Time-dependent quantum mechanics problems are usually addressed using time-dependent perturbation theory, adiabatic or sudden approximations as well as several

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numerical techniques. It is highly desirable, however, to obtain exact analytical solutions to given problems, especially in cases when the approximate methods may be inadequate to describe detailed aspects of the solutions or when numerical treatment does not explicitly reveal their mathematical properties at very large times. Recently, there has been increasing interest in obtaining exact analytical solutions to the time-dependent Schrödinger equation since they can be used to study certain physical systems such as quantum dots, Bose-Einstein condensates, unstable composite particles and many others. Burrows and Cohen [11] have developed exact solutions for a double-well quasi-harmonic potential model with a time-dependent dipole field. Cavalcanti, Giacconi and Soldati [2] have solved the problem of decay from a point-like potential well in the presence of a uniform field and have indicated that, due to an infinitely large number of resonances, there may be deviations from the naively expected exponential time-dependence of the survival probability.

The equivalence of exponential decay of a given energy eigenstate with Fermi’s golden rule when the final density of states is energy-independent and with the Breit-Wigner resonance curve has been long known in quantum mechanics [3, 4]. Dullemond [5] has verified this fact in a simple but exactly solvable model and found that if final-state energy-dependence is introduced into this model a non-exponential decay pattern will dominate at large times. Petridis et al., [6] have studied a variety of systems in which the initial wave function is mostly or entirely set in a finite potential well and have observed rich behaviour, including non-exponential decay into the continuum. Non-exponentiality for monotonically decreasing survival probabilities at large times, though, can be strictly proven only if exact analytical solutions are obtained. Specific systems that may exhibit non-exponential decay include systems with non-local interactions [7], certain closed many-body systems [8], quasi-particles in quantum dots [9], polarons [10], and non-extensive systems [11].

In this article a method for developing analytical solutions to the time-dependent Schrödinger equation is presented. The method is applied to a time-independent potential, consisting of an infinite wall and a repulsive delta function. In addition to the mathematical interest that this potential exhibits it is also applicable to a variety of quantum systems undergoing decay. A wavefunction that is an exact solution subject to the boundary conditions is obtained and used to analytically calculate the probability for finding the particle inside the potential well at any time. A generalization of the asymptotic time behaviour to all square-integrable wavefunctions is obtained.

2 The proposed method

The method consists of the following steps: (a) The time-independent solutions to Schrödinger equation are found subject to the boundary conditions of the problem. These are stationary solutions, that is energy eigenfunctions, that span the Hilbert space of the given Hamiltonian. (b) Since any finite or infinite, discrete or continuous linear combination of the stationary solutions (base functions) is also a solution
belonging to the given Hilbert space, as long as it is square-integrable, exact analytical solutions can be developed by a convolution of the eigenfunctions with energy-dependent spectral functions multiplied by the standard oscillator time-dependence of the stationary states. It is, obviously, necessary that the convolution integral over the energy converge. This convergence as well as the square-integrability (normalizability) of the resulting wave function are verified. (c) The survival probability, i.e., the probability for finding the particle inside the potential well is calculated and its properties are studied analytically.

3 Infinite wall and delta-function potential

The problem to be considered is defined by the one-dimensional repulsive potential,

\[ V(x) = \infty, \quad -\infty \leq x \leq 0 \]  \quad and \quad \[ V(x) = V_0 \delta(x - L), \quad 0 < x \leq \infty, \]  \quad (1)

with \( L > 0 \) and \( V_0 > 0 \). The steps outlined in the previous section are followed.

(a) The solutions to the time-independent Schrödinger equation,

\[ -\frac{1}{2} \frac{d^2 \Psi_E(x)}{dx^2} + V(x)\Psi_E(x) = E \Psi_E(x), \]  \quad (2)

(with particle mass \( m = 1 \), \( \hbar = 1 \) and \( E \geq 0 \)) are,

\[ \Psi^{(0)}_E(x) = 0, \quad -\infty \leq x \leq 0 \]  \quad (region "0"),

\[ \Psi^{(I)}_E(x) = C_1 \sin(px), \quad 0 \leq x \leq L \]  \quad (region "I"),

\[ \Psi^{(II)}_E(x) = C_2 \sin(px) + C_3 \cos(px), \quad L \leq x \leq \infty \]  \quad (region "II"),

where \( p = \sqrt{2E} \) and \( C_{1,2,3} \) are constants in \( x \). These functions obey the boundary conditions

\[ \Psi^{(I)}_E(L) = \Psi^{(II)}_E(L), \]  \quad (6)

\[ \frac{d\Psi^{(I)}_E}{dx}(L) - \frac{d\Psi^{(II)}_E}{dx}(L) = 2V_0 \Psi^{(I)}_E(L), \]  \quad (7)

while the boundary conditions at \( x = 0 \) are automatically satisfied. The solution is not required to vanish at infinity since functions that do not vanish at large \( x \) can still be solutions to the time-dependent problem. Selecting \( C_1 \) as the overall normalization constant the boundary conditions at \( x = L \) yield

\[ C_2 = C_1 \left[ 1 + \frac{2V_0}{p} \sin(pL) \cos(pL) \right], \]  \quad (8)

\[ C_3 = -C_1 \left( \frac{2V_0}{p} \right) \sin^2(pL), \]  \quad (9)
rendering $C_2$ and $C_3$ functions of the energy. The choice of $C_2$ or $C_3$ as the normalization constant would introduce an energy-dependence in $C_1$ and would effectively amount to different spectral functions.

The obtained linearly independent energy eigenfunctions are orthogonal under the inner product

$$ (\psi_1, \psi_2) = \int_0^L \psi_1^*(x) \psi_2(x) \, dx + \lim_{\epsilon \to 0} \int_L^\infty e^{-\epsilon(x-L)} \psi_1^*(x) \psi_2(x) \, dx, \quad (10) $$

with all wavefunctions in the defined Hilbert space identically vanishing for $x \leq 0$. The orthogonality relation is

$$ (\Psi_E, \Psi_{E'}^*) = w(E) \delta(p - p'), \quad (11) $$

where $p = \sqrt{2E}$, $p' = \sqrt{2E'}$ and

$$ w(E) = \frac{\pi}{2} \left[ |C_2(E)|^2 + |C_3(E)|^2 \right] \quad (12) $$

$$ = |C_1|^2 \frac{\pi}{2p^2} \left[ p^2 + 2V_0^2 - 2V_0^2 \cos (2pL) + 2pV_0 \sin (2pL) \right]. $$

The Dirac $\delta$-function representation used is

$$ \delta(x) = \lim_{\epsilon \to 0} \frac{1}{\pi \epsilon} \frac{1}{x^2 + \epsilon^2}. \quad (13) $$

(b) The solution to the time-dependent Schrödinger equation,

$$ -i \frac{\partial \psi(x,t)}{\partial t} = -\frac{1}{2} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \psi(x,t), \quad (14) $$

can be written as the energy-convolution integral,

$$ \psi(x,t) = \int_0^\infty \phi(E) \Psi_E(x) e^{-iEt} \, dE, \quad (15) $$

with $\phi(E)$ a spectral function such that this integral is convergent for all $x$ and all $t$ and the resulting wavefunction is square-integrable. Square-integrability of $\psi(x,t)$ also requires $E$ to be real. The overall normalization constant is, then, calculated from

$$ \int_0^\infty \psi^*(x,t)\psi(x,t) \, dx = 1. \quad (16) $$

The choice of spectral function

$$ \phi(E) = e^{-K^2E}, \quad (17) $$

with $K$ a positive constant, produces a convergent energy-convolution integral and a wavefunction that is square-integrable even without the presence of the convergence.
factor that appears in eq. (10). These integrals can be evaluated analytically and in closed form. The time-dependent solution is, then,

\[ \psi^{(0)}(x, t) = 0, \quad (18) \]

\[ \psi^{(I)}(x, t) = C_1 \sqrt{\frac{\pi}{2}} x e^{-\frac{x^2}{2(K^2 + it)}} (K^2 + it)^{-3/2}, \quad (19) \]

\[ \psi^{(II)}(x, t) = C_1 \sqrt{\frac{\pi}{2}} e^{-\frac{x^2}{2K^2}} (K^2 + it)^{-3/2} \]

\[ \left[ e^{2(K \pi + it)} (K^2 + it)V_0 + e^{\frac{i-2L^2}{2K^2}it^2} (-K^2V_0 - itV_0 + x) \right], \quad (20) \]

where

\[ C_1 = \left[ \frac{\pi^{3/2}}{8K^3} + \frac{e^{-\frac{L^2}{K^2}} L\pi^{3/2}V_0}{2K^3} + \frac{\pi^{3/2}V_0^2}{2K} - \frac{e^{-\frac{L^2}{K^2}} \pi^{3/2}V_0^2}{2K} \right]^{-1/2} \quad (21) \]

is the overall normalization factor obtained by means of eq. (16).

(c) The probability density \( \rho = \psi^*(x, t)\psi(x, t) \) can be calculated for the interior (region I) and the exterior (region II) of the potential well. It is presented in Fig. 1 at six times starting from \( t = 0 \), in increasing order. The initial wave function is not entirely localized inside the well. As time progresses the wavefunction spreads and tunnels through the potential barrier in both directions. The interference of the wave that propagates outwards through the barrier and the wave that is outside creates the observed ripples. Inside the well there are no ripples because the wavefunction is forced to be odd in \( x \), having a node at \( x = 0 \). The centroid of the probability density in region II at \( t = 0 \) is always located at \( 2L \), regardless the value of \( K \).

The survival probability is, then, calculated as

\[ P_{in}(t) = \int_0^L \psi^*(x, t)\psi(x, t) \, dx. \quad (22) \]

This yields the closed-form result

\[ P_{in}(t) = C_1^2 \left[ \frac{\pi^{3/2}}{8K^3} \text{Erf} \left( \frac{KL}{\sqrt{K^4 + t^2}} \right) - \frac{2\pi KL}{8K^3\sqrt{K^4 + t^2}} e^{-\frac{K^2t^2}{K^4 + t^2}} \right]. \quad (23) \]

A plot of the survival probability versus time is given in Fig. 2. \( P_{in}(0) \) is controlled by \( K \) and approaches an upper limit as \( L \) increases at fixed \( K \). For example, this limit is equal to 0.9615 for \( K = 0.1, 0.5 \) at \( K = 0.5 \) and 0.1468 at \( K = 1.2 \). It decreases as \( K \) increases, i.e., as the momentum spectrum becomes sharper. On the other hand the decay becomes slower as \( K \) increases. The expansion of \( P_{in} \) in inverse powers of time includes only odd terms with alternating signs. At large times the leading term, that has a positive sign, is proportional to \( t^{-3} \), a clearly non-exponential behaviour.
Figure 1: The probability density for a potential consisting of an infinite wall and a repulsive delta function and using a spectral function that is exponential in the energy at six increasing times (from the upper left to the lower right panel, $t = 0.0, 0.3, 0.6, 0.9, 1.2, 1.5$). In this plot $L = 3$, $V_0 = 1$ and $K = 1/2$. 
Figure 2: The survival probability for a potential consisting of an infinite wall and a repulsive delta function and using a spectral function that is exponential in the energy versus time (solid line). In this plot $L = 3$, $V_0 = 1$ and $K = 1/2$. The dashed line represents the exponentially decaying function, $f(t) = a \exp(-bt)$, fitted to data points, calculated from the actual solution, in the range $t = 2$ to $4$. The $\chi^2$ per degree of freedom is of order $10^{-6}$.

4 Corrections to the exponential decay law

The law governing the decay of physical systems is typically assumed to be a simple exponential time-dependence of the number $N(t)$ of the systems that have not decayed until time $t$, i.e., $N(t) = N(0) \exp(-\lambda t)$, where $\lambda$ is the decay constant. As mentioned earlier this simple law is consistent with the Breit-Wigner curve and Fermi’s golden rule if the final density of states is energy independent. It refers to the survival probability of a given initial energy eigenstate. In the system studied here the initial state is not an eigenstate of the energy. If a very large number of systems is assumed to be initially described by $\psi(x, 0)$ and a system is said to have decayed if the particle has exited the potential well, then the number of surviving systems is proportional to the probability $P_{\text{in}}$, i.e.,

$$\frac{N(t)}{N(0)} = \frac{P_{\text{in}}(t)}{P_{\text{in}}(0)}. \quad (24)$$

The differential decay law is

$$dN = -\lambda(t)N(t) \, dt, \quad (25)$$

where, $\lambda$ is, in general, dependent on time. Substitution from eq. (24) gives

$$\lambda(t) = -\frac{1}{P_{\text{in}}} \frac{dP_{\text{in}}}{dt} = -\frac{d}{dt} \ln(P_{\text{in}}(t)). \quad (26)$$
Figure 3: The decay parameter $\lambda$ for a potential consisting of an infinite wall and a repulsive delta function and using a spectral function that is exponential in the energy versus time. In this plot $L = 3$ and $K = 1/2$. There is no dependence on $V_0$.

In the case studied, eq. (23) yields

$$\lambda(t) = \frac{4e^{-z^2}z^3t}{(K^4 + t^2)[-2ze^{-z^2} + \sqrt{\pi}\text{Erf}(z)],}$$

where $z = KL/\sqrt{K^4 + t^2}$. This function is plotted versus time in Fig. 3.

The decay parameter $\lambda$ peaks later in time and has a smaller maximum value as $K$ or $L$ increase but does not depend on $V_0$. The expansion of $\lambda$ in inverse powers of time includes only odd terms with alternating signs. At large times the leading term, that has a positive sign, is proportional to $t^{-1}$, affirming the non-exponential behaviour. At very large times the change of $\lambda$ with time is rather slow. A fit to $P_{in}$ at large times with an exponential curve in a finite time interval (as it is done in experiments) gives a very small value of $\chi^2$ per degree of freedom (of order $10^{-6}$) so that the distinction between $P_{in}$ at large times and a simple exponential decay function is numerically minute (Fig. 2).

## 5 Generalization

Exact, closed-form, analytical solutions to the time-dependent Schrödinger equation for the potential consisting of an infinite wall and a repulsive delta function can be and have been obtained for other spectral function choices. For example, the choice

$$\phi(E) = -i \frac{[1 - \cos \left( \frac{L}{2} \sqrt{2E} \right)]}{2E \sqrt{\pi L}}$$

(28)
yields a square-integrable wavefunction. In the absence of the delta function at \( x = L \) this would produce an effectively square density pulse at \( t = 0 \) located between \( x = 0 \) and \( x = L/2 \). Due to the actual boundary conditions at \( x = L \) this spectral function also produces a cusp centered at \( x = 2L \). The survival probability is readily expressible in terms of Fresnel sine and cosine integrals. Its asymptotic large time behaviour is still \( t^{-3} \).

A question that naturally arises at this point is whether the asymptotic time behaviour can be generalized to other possible solutions to this problem. There is a one-to-one correspondence between spectral functions and square-integrable wavefunctions. This can be seen upon projecting the wavefunction at \( t = 0 \) on an energy eigenfunction and employing the orthogonality condition of eq. (11):

\[
\phi(E) = \frac{1}{w(E)} \int_0^\infty \Psi^*_E(x)\Psi(x,0) \, dx. \tag{29}
\]

Given an initial wavefunction the corresponding spectral function can, in principle, be constructed. Schrödinger’s time-dependent equation then produces the wavefunction at any later (or earlier) time.

Convergence of the energy convolution integral in region (II) requires that the spectral function be finite at \( E \to 0 \). In addition, in order for \( \Psi(x,t) \) to be square-integrable, \( \phi(E) \) must vanish at large energies. This requirement can be made precise by inserting eq. (15) into eq. (16) and applying eq. (11) to obtain

\[
\int_0^\infty w(E)|\phi(E)|^2 \, dE = 1. \tag{30}
\]

Inspection of the function \( w(E) \), given in eq. (12), leads to the conclusion that \( |\phi(E)| \) must vanish at infinity faster than \( 1/\sqrt{E} \) due to a constant term in \( w(E) \).

Assuming that \( \phi(E) \) satisfies the convergence conditions, its contribution to the energy convolution integral giving \( \Psi^{(I)}(x,t) \) comes mostly from low energies. Then at any \( x \) in region (I) the wavefunction can be approximated as

\[
\Psi^{(I)}(x,t) \approx C_1 \phi(0) \int_0^{E_{\text{max}}(t)} \sqrt{2E} \, x \, e^{-iEt} \, dE. \tag{31}
\]

The upper limit of the integration is chosen as follows: the factor \( \exp(-iEt) \) oscillates more rapidly with the energy as \( t \) increases. At very large times these oscillations eventually lead to a vanishing contribution to the integral. Therefore, the integral can be cut off at a point \( E_{\text{max}}(t) \) whose first order term in the expansion in powers of \( 1/t \) is \( y_{\text{max}}/t \), where \( y_{\text{max}} \) is constant in \( t \). At low energies \( \phi(E) \) is replaced by its (finite) value at \( E = 0 \) and the sine function is substituted by its argument at a given \( x \). Then, the variable change \( y = Et \) yields

\[
\psi^{(I)} \approx C_1 \phi(0) \, t^{-3/2} \int_0^{y_{\text{max}}} \sqrt{2y} \, e^{-iy} \, dy. \tag{32}
\]
For small $y_{\text{max}}$ the integral is approximately $\sqrt{2} \left[ \left( \frac{2}{3} \right) y_{\text{max}}^{3/2} - i \left( \frac{2}{5} \right) y_{\text{max}}^{5/2} \right]$. The wavefunction in region (I) is to the first non-vanishing order

$$\Psi^{(I)}(x, t) \approx C_1 \phi(0) \, x \, M \, t^{-3/2}, \quad (33)$$

where $M$ is a constant and the survival probability decreases with time as $t^{-3}$. Therefore, in order for the wavefunction to be square-integrable, the spectral function must be finite at $E \to 0$ and decrease at large $E$ faster than $1/\sqrt{E}$ and then necessarily the survival probability asymptotically decreases as the inverse cube of time.

This argument can be extended to any finite value of $x$ including region (II) since the coefficients $C_2$ and $C_3$ are at most of $O(1)$ for small $E$. Therefore, the integral of the probability density over any finite range of $x$ is finite (even without the convergence factor present in eq. (10)) and it decreases asymptotically as $t^{-3}$.

The constant $M$ in eq. (33) can be exactly evaluated if $\phi(E)$ decreases at large $E$ faster than $1/E$. Then if $\phi(E)$ is analytic in the fourth quadrant of the complex $E$-plane the contour integral of $\phi(E) \sin (x \sqrt{2E}) \exp(-iEt)$ along a closed path, consisting of the positive real axis from $R$ to 0, the negative imaginary axis from 0 to $-iR$ and a quarter-circle, $\Gamma$, of radius $R$, is zero. The integral along $\Gamma$ is bounded by a constant times $1/R^k$ with $R = |E|$ and $k > 1$ and, consequently, vanishes in the limit $R \to \infty$. Then the integration over the real axis gives the same result as that over the imaginary axis. The variable change $E = -iy$ with $y$ real, then, yields

$$\Psi^{(I)}(x, t) = -i C_1 \int_0^\infty \phi(-iy) \sin \left( x \sqrt{-2iy} \right) e^{-yt} \, dy. \quad (34)$$

For large times only small values of $y$ contribute to the integral. The spectral function is substantially different from zero only close to the origin and can be replaced by $\phi(0)$ and be pulled out of the integral while the sine function can be approximated by its argument in a finite range of $x$. The remaining integral is easily evaluated as a gamma function and gives

$$\Psi^{(I)}(x, t) \approx C_1 \phi(0) \, x \, e^{-i3\pi/4} \sqrt{\pi/2} \, t^{-3/2} \quad (35)$$

confirming the earlier result.

The survival probability, $P_{in}$, calculated thus far refers to the presence of the particle inside the potential well. As it has been shown in the previous section the spectral function of eq. (17) produces non-zero probability density outside the well at $t = 0$ for $K > 0$. If the "interior" of the well is defined to extend to $x$ much larger than $2L$ (without moving the delta function from $x = L$) then at $t = 0$ the probability to find the particle "inside" can be arbitrarily close to unity. Specifically the modified survival probability $P_{in}(4L)/(t)$ can be defined by extending the integral of eq. (22) to $x = 4L$. This integral is then evaluated analytically and plotted in Fig. 4 as a function of time. As predicted and verified by an expansion of $P_{in}(4L)$ in inverse powers of time, its asymptotic time dependence is $t^{-3}$. An interesting feature of this plot is the presence of a step-wise behaviour which can be attributed to interference between waves moving in opposite directions.
Figure 4: The modified survival probability for a potential consisting of an infinite wall and a repulsive delta function and using a spectral function that is exponential in the energy versus time (solid line). In this plot $L = 3$, $V_0 = 1$ and $K = 1/2$. The step-wise behaviour is due to interference of waves moving in opposite directions.

6 Conclusions and perspectives

A method has been proposed to solve the time-dependent Schrödinger equation utilizing the much more easily obtained time-independent solutions for a given Hamiltonian. It has been applied to the case of a potential consisting of an infinite wall and a repulsive delta function. An exact, analytical, normalized solution has been obtained in closed form. The survival probability, which is also analytically calculated, exhibits a non-exponential behaviour. At large times it decays approximately as $t^{-3}$. It was shown that this behaviour pertains to all square-integrable wavefunctions that are solutions to this problem. To ensure square-integrability the spectral function must be finite at $E \rightarrow 0$ and decrease to 0 at large energies faster than $1/\sqrt{E}$. With the appropriate choice of spectral functions which, due to linear independence need not be the same for waves propagating in different directions, the method could be applied to a variety of potentials. It is also of great interest to develop solutions for the time-dependent relativistic Dirac equation since these are more appropriate to describe the decay of mesons into light leptons.

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