REAL TIME QUANTUM TUNNELING

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(received: 15 November 2014;
accepted: 10 January 2015; published online: 16 February 2015)

Abstract: The time evolution of the probability and current densities stemming from an initial state of a particle in the form of a wave packet on the left hand side of a square barrier is studied. In particular, the space distribution at a given time of the above densities is given. Furthermore, the evolution in time at the entrance and exit of the barrier is given. The numerical results show repeated reversal in the current density at the barrier entrance, while being unidirectional at the exit. However, the probability entering the barrier over a long time equals the corresponding probability exiting the barrier. Owing to the fact that the wave packet expands on both of its sides, as time goes by, it is possible to have transmission even if the particle's initial momentum points away from the barrier. The effect, in question, becomes evident in a diagram for the transmission coefficient in terms of the particle initial momentum, over a relatively small region.

Keywords: quantum tunneling, square barrier propagator, transmission coefficient

1. Introduction

In the present work we deal with time dependent quantum tunneling utilizing a set up involving a particle, initially in wave packet state, located on the left hand side of a one dimensional (1D) square barrier, towards which approaches or moves away. The wave packet's centre and spread are such that its overlap with the barrier is extremely negligible.

In the literature one encounters papers dealing with scattering of a wave packet by a square barrier. In [1] spatial probability density is reported at various times via numerical solution of the relevant Schrödinger equation. Furthermore the probability density in momentum representation [2] is obtained analytically. Nevertheless the time evolution of the corresponding wave function is based on superposition of degenerate eigenfunctions, namely, the one employed in the corresponding plane wave scattering by a square barrier. However, for obtaning a complete set of eigenfucntions the degenerate ones are required.

Presently, we employ a particular scheme leading to detailed results concerning, not only, the probability, but also, the current densities for the barrier incoming, or outgoing, particle, both time and space-wise. Use is made of the associated propagator through a complete set of eigenfunctions. For a form of the propagator in the case of a particle under the influence of a square barrier ($\times 1/i\hbar$), via Green's function, see [3]. A further way for obtaining tunneling propagators can be seen in [4].

As far as applications are concerned from the study of wave packet transmission through tunneling barriers the reader can find in [5]. Essentially they have to do with tunneling times within the femptosecond region.

In Section 2 we obtain expressions for the transmission probability utilizing current densities at the barrier entrance or exit as they evolve in time over extremely long times, or the spatial distribution of the probability density passed the barrier at extremely long time. In Section 3 the square barrier propagator, necessary for determining the wave function employed in Section 2, is obtained utilizing a relevant complete set of eigenfunctions. In Section 4 we deal with numerical results providing spatial distributions of probability and current densities at given times, as well as their time evolution at the barrier boundaries. Finally, a graph for the transmission coefficient in terms of the mean momentum of the initial wave packet is provided. Section 5 deals with conclusions.

2. Probability and current densities

Presently, we consider a (1D) square barrier with potential energy

$$U(x) = u_o[\Theta(x+a) - \Theta(x-a)] \tag{1}$$

where Θ stands for the step function, u_o the barrier height, $a > 0$ indicating the barrier exit, while barrier entrance lies at $x = -a$. As pointed out earlier, the barrier is approached by a particle, initially in a wave packet state

$$\Phi(x) = \frac{1}{(2\pi s^2)^{1/4}} \exp\left[-\frac{1}{4s^2}(x-x_o)^2 + \frac{i}{\hbar}p_o(x-x_o)\right] \tag{2}$$

where x_o, p_o and s are respectively the wave packet centre, mean momentum, and mean spread.

Under the circumstances, in the course of time the wave function, stemming from the wave packet, expands on either side, but faster in the direction of the mean momentum, p_o. At some later time the right hand side (RHD) edge of the evolving wave function reaches the barrier entrance ($x = -a$) and the particle receives, further, the barrier's influence. In the ensuing time the wave function edge reaches the barrier exit ($x = a$) and proceeds crossing the barrier.

Once the evolving wave function, say, $\Psi(x,t)$, is available we can obtain the probability and current densities, ρ and J, both time and space-wise, as

$$\rho(x,t) = |\Psi(x,t)|^2, \quad J(x,t) = \frac{\hbar}{m}\Im\left[\Psi^*(x,t)\frac{\partial}{\partial x}\Psi(x,t)\right] \tag{3}$$

m being the particle's mass.

As we shall see in Section 4 the current density at the barrier entrance, $J(-a,t)$ initially flows into the barrier, subsequently current enters and gets out of the barrier at the entrance, repeatedly, and eventually after quite a time tends to zero. In what concerns the current density at the barrier exit, $J(a,t)$, once current begins exiting the barrier it follows the same direction, and after quite a long time, essentially, ceases, while the barrier region becomes probability empty. Beyond this extremely long time the probability density, $\rho(x,t)$, gets stabilized, and essentially becomes zero beyond very large distances on either side of the barrier.

Considering that the transmission coefficient, T_c, is provided by the fraction of probability installed beyond the barrier exit after a long time, say, t_o, when the probability and current densities stabilize, we have:

$$T_c = \int_0^{t_o} J(-a,\tau)d\tau = \int_0^{t_o} J(a,\tau)d\tau \tag{4}$$

Alternatively, on the basis of the discussion following (3), T_c can be obtained via the spatial probability density, as

$$T_c = \int_0^{l_2} \rho(x,t_o)dx \tag{5}$$

l_2 being extremely large so as ρ at time t_o becomes essentially zero.

Clearly, we have

$$\int_{l_1}^{-a} \rho(x,t_o)dx = 1 - T_c \tag{6}$$

where $l_1 < 0$ for which $x < l_1 \rho(x,t_o)$ becomes essentially zero. Expressions (4), (5), (6) are practically accurate, but for absolute precision, t_o, l_2 must go to ∞ and l_1 to $-\infty$.

The procedure for obtaining the required wave function $\Psi(x,t)$ stemming from the initial wave packet, $\Phi(x)$, requires solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\Psi(x,t) \tag{7}$$

under the condition

$$\Psi(x,0) = \Phi(x) \tag{8}$$

This can be attained through the propagator, $K(xt|x'0)$, of Schrödinger Equation (7), from which the required wave function is obtained as

$$\Psi(x,t) = \int_{-\infty}^{\infty} K(xt|x'0)\Phi(x')dx' \tag{9}$$

As is well known $K(xt|x'0)$ solves Schrödinger's equation and obeys the initial condition

$$K(xt|x'0) \to \delta(x-x'), \text{ as } t \to 0 \tag{10}$$

which enables condition (8) to be satisfied. Details for obtaining the propagator, in question, follow in section 3 as well as explicit expression for $\Psi(x,t)$.

Prior to closing the present section it would be useful to point out that $\Phi(x)$ can take the form:

$$\Phi(x)=\int_0^\infty G(k)[f(k)+f(-k)]dk \tag{11}$$

where:

$$G(k)=\left(\frac{s}{\pi}\right)^{1/2}\frac{1}{(2\pi)^{1/4}}\exp(-s^2k^2),\quad f(k)=\exp[i(k+\frac{1}{\hbar}p_o)(x-x_o)] \tag{12}$$

The above structure form of the wave packet leads to the possibility of having transmission in case $p_o<0$. As a matter of fact for $k>|p_o|/\hbar$ we have a mixture of incoming and outgoing plane waves, i.e. $\exp[i(k-\frac{|p_o|}{\hbar})(x-x_o)]+\exp[-i(k+\frac{|p_o|}{\hbar})(x-x_o)]$, both with amplitude $G(k)$, given in (12). In case $|p_o|$ is sufficiently small the incoming wave is still effective for transmission, although small. However, for $|p_o|$ large the amplitude $G(k)$ for which it is possible to have an incoming wave i.e. $\exp[i(k-\frac{|p_o|}{\hbar})(x-x_o)]$ for $k>|p_o|/\hbar$ becomes too small for both incoming and outgoing waves. Thus, transmission possibility gets disallowed.

3. Square Barrier Propagator

The problem we are faced with is to obtain the propagator of Schrödinger Equation (7) for which the potential energy, $U(x)$, is provided in three regions, 1, o, 2, namely, (1) for $x<-a$, (o) for $-a\le x\le a$ and (2) for $x>a$. Under the circumstances the various eigenfunctions associated with the equation, in question, are expressed for each region separately.

For obtaining the relevant propagator we require a complete set of normalized eigenfucntions. We begin with the following symmetric and antisymmetric solution of Schrödinger Equation (1) valid for region (1), (o) and (2) as in (13)–(14), and denoted by Y_{is} and Y_{ia} ($i=1$, o, 2) respectively and given by

$$\begin{aligned}
Y_{1s}&=\cosh(Ka)\cos[k(x+a)]-\frac{K}{k}\sinh(Ka)\sin[k(x+a)]\\
Y_{os}&=\cosh(Kx)\\
Y_{2s}&=\cosh(Ka)\cos[k(x-a)]+\frac{K}{k}\sinh(Ka)\sin[k(x-a)]
\end{aligned}\tag{13}$$

$$\begin{aligned}
Y_{1a}&=-\sinh(Ka)\cos[k(x+a)]+\frac{K}{k}\cosh(Ka)\sin[k(x+a)]\\
Y_{oa}&=\sinh(Kx)\\
Y_{2a}&=\sinh(Ka)\cos[k(x-a)]+\frac{K}{k}\cosh(Ka)\sin[k(x-a)]
\end{aligned}\tag{14}$$

where $K=\sqrt{2mu_o/\hbar^2-k^2}$, and k stands for the quantum number associated with the wave function solutions (13)–(14). Clearly, (13) and (14) satisfy the continuity conditions for the wave function and its derivative at the barrier boundaries. In case the three regions cover the interval $(-\infty,\infty)$ k is continuous. It is also positive, on accounts of the fact Y_{is} and Y_{ia} for $k<0$ are duplicated. Furthermore, the energy eigenvalue is given by $E_k = \hbar^2 k^2/2m$ for either the symmetric or antisymmetric case.

Let us, now, proceed to obtain the normalizing factors A_s and A_a of the wave functions given in (13) and (14), respectively. To this extent, we consider initially a region ranging from $-L$ to L, $(L>0)$. In this case k becomes discrete, which for extremely large L approaches to a very high degree the expression $k=(\pi/L)n$ $(n=1,2,3,\ldots)$. Under these circumstances the expression for both symmetric and antisymmetric solutions of Schrödinger's Equation (7) acquire periodic boundary conditions with period L.

We, now, proceed to obtain normalization coefficients, A_s and A_a for a given L. We have:

$$A_s = \left(\int_{-L}^{-a} Y_{1s} Y_{1s}^* dx + \int_{-a}^{a} Y_{os} Y_{os}^* dx + \int_{a}^{L} Y_{2s} Y_{2s}^* dx \right)^{-1/2} \tag{15}$$

$$A_a = \left(\int_{-L}^{-a} Y_{1a} Y_{1a}^* dx + \int_{-a}^{a} Y_{oa} Y_{oa}^* dx + \int_{a}^{L} Y_{2a} Y_{2a}^* dx \right)^{-1/2} \tag{16}$$

It should be noted that the first and third integrals in (15) and (16) are equal. Although, the integrations, above, can be performed analytically they result in lengthy expressions, and we shall avoid stating them. We note only that A_s and A_a depend on k and L, and are real quantities. The above expressions for A_s and A_a can be employed, in case of very large L for obtaining the required propagator. For this purpose we need the normalized eigenfunctions, which take the form:

$$\Psi_{is}(k,x) = A_s(k,L) Y_{is}(k,x) \tag{17}$$

$$\Psi_{ia}(k,x) = A_a(k,L) Y_{ia}(k,x) \tag{18}$$

x in region i $(i=1,o,2)$.

The propagator for x in region i and x' in region j can be expressed as:

$$K_{ij}(xt|x'0) = \frac{L}{\pi} \int_0^\infty \left[A_s^2 Y_{is}(k,x) Y_{js}^*(k,x') + A_a^2 Y_{ia}(k,x) Y_{ja}^*(k,x') \right] \cdot \exp\left(-i \frac{\hbar k^2}{2m} t \right) dk \tag{19}$$

It should be noted that the expressions LA_s^2/π and LA_a^2/π in (19) essentially tend to zero beyond, not a very large, value of k. So, one can obtain sufficiently accurate results for appropriate finite range of integration over k.

Proceeding to the limit $L \to \infty$ in (19) we have for the propagator the expression

$$K_{ij}(xt|x'0) = \int_0^\infty \left[F_s(k)Y_{is}(k,x)Y^*_{js}(k,x') + F_a(k)Y_{ia}(k,x)Y^*_{ja}(k,x')\right] \cdot \exp\left(-i\frac{\hbar k^2}{2m}t\right)dk \tag{20}$$

where, F_s and F_a in (20) are given by

$$F_s(k) = \lim_{L\to\infty} \frac{L}{\pi} A_s^2(k,L) = \frac{1}{\pi} \frac{k^2}{k^2\left|\cosh(Ka)\right|^2 + \left|K\right|^2 \left|\sinh(Ka)\right|^2} \tag{21}$$

$$F_a(k) = \lim_{L\to\infty} \frac{L}{\pi} A_a 2(k,L) = \frac{1}{\pi} \frac{k^2}{\left|K\right|^2\left|\cosh(Ka)\right|^2 + k^2 \left|\sinh(Ka)\right|^2} \tag{22}$$

(20) provides the propagation for x and x' in the whole region from $-\infty$ to ∞.

Prior to closing this section we shall provide expression for the wave function $\Psi_i(x,t)$ stemming from the initial wave packet $\Phi(x)$ given in (2) for the regions $(i = 1, o, 2)$. As pointed out, earlier, the wave packet is located in region (1), while in the other regions is essentially zero. On the basis of essentially the non – zero extent of $\Phi(x)$ in only the region (1), the required evolving wave function $\Psi_i(x,t)$ in the regions $(i = 1, o, 2)$ can be obtained as

$$\Psi_i(x,t) = \int_{-\infty}^{-a} K_{i1}(xt|x'0)\Phi(x')dx' \tag{23}$$

Since, $\Phi(x)$ for $x > -a$ Is practically zero the integral in (23) can be extended in the range from from $-\infty$ to ∞. Thus, denoting by Φ_{1s} and Φ_{1a} the integrals

$$\Phi_{1s}(k) = \int_{-\infty}^{\infty} Y_{1s}(k,x')\Phi(x')dx' \tag{24}$$

$$\Phi_{1a}(k) = \int_{-\infty}^{\infty} Y_{1a}(k,x')\Phi(x')dx' \tag{25}$$

we obtain for $\Psi_i(x,t)$ for $(i = 1, o, 2)$ the result

$$\Psi_i(x,t) = \int_0^\infty \left[F_s(k)\Phi_{1s}(k)Y_{is}(k,x) + F_a(k)\Phi_{1a}(k)Y_{ia}(k,x)\right]\exp(-i\frac{\hbar k^2}{2m}t)dk \tag{26}$$

Having obtained the evolving wave function stemming from the initial wave packet we can employing (3) obtain the probability and current densities time- and space-wise.

4. Numerical results

In this section we present results on the basis of which one can form a picture of the spatial distribution for the probability and current densities at given times, as well as their corresponding time evolution at the barrier entrance and exit. Furthermore, we obtain the transmission coefficient as a function of the mean momentum carried by the wave packet with barrier parameters (u_o, a, s), given in data in common, which follow.

In order to proceed numerically it would be helpful to introduce as unit of energy $E_u = 0.1eV$ $(= 1.601917 \cdot 10^{-13}\,\text{erg})$. On the basis of this unit together with the carrier particle mass, m, we form the units of time, length, velocity, and momentum correspondingly as:

$$T_u = \frac{\hbar}{E_u}, \quad L_u = \frac{\hbar}{\sqrt{mE_u}}, \quad V_u = \frac{L_u}{T_u}, \quad P_u = m\frac{L_u}{T_u} \tag{27}$$

Using for m the electron mass, $m = 9.109558 \cdot 10^{-28}\,\text{g}$, and $\hbar = 1.054559 \cdot 10^{-27}\,\text{erg·s}$ for Planck's constant, the units in (27) have the following values: $T_u = 6.58198 \cdot 10^{-15}$, $s = 6.58198\,\text{fs}$, $L_u = 8.72901 \cdot 10^{-8}\,\text{cm}$, $V_u = 1.32262 \cdot 10^{7}\,\text{cm/s}$, $P_u = 1.20811 \cdot 10^{-20}\,\text{g·cm/s}$. It should be noted that the choice of $E_u = 0.1\,\text{eV}$ derives from the usual value of barrier height, being on the order of a few $0.1\,\text{eV}$. Clearly, if we employed effective mass for m there would result change in the units of length, velocity and momentum, while the time unit would not be affected.

The above system of units enables dealing with dimensionless quantities, just by setting in Schrödinger's Equation (7) $\hbar = 1$, $m = 1$. The various dimensional results are obtained from the resulting dimensionless quantities times their associated units, given in (27). Utilizing the procedure, in question, we can obtain via (26) the required wave function $\Psi_i(x,t)$ from which we derive probability and current densities, ρ and J, through (3), as well as transmission coefficient, T_c, using either (4) or (5).

In the ensuing results we make use of data in common with regard to the barrier potential being $u_o = 5E_u$, $a = 2L_u$, while for the initial wave function $s = 0.2L_u$. The parameters x_o and p_o for the wave packet can be varied and are given in the corresponding figure captions.

The figures below refer to the probability and current densities. In particular, Figure 1(a) depicts initial probability density space distribution (solid curve) as well as the form it takes after a short time, $1T_u$, (dashed curve). Figure 1(b) provides the corresponding spatial distributions of the current densities. Subsequently, Figures 2(a), (b) show correspondingly probability and current densities at $t = 8T_u$.

Results concerning time evolution of probability and current densities at the barrier entrance are presented in Figures 3(a), (b), while corresponding results are shown in Figures 4(a), (b) at the exit. In what concerns the current density at the entrance there appears successive change in the current direction, while at the exit current gets out continuously. Evidently, the more away from barrier the location of the initial wave packet the longer it takes for the probability and current densities to start and get established.

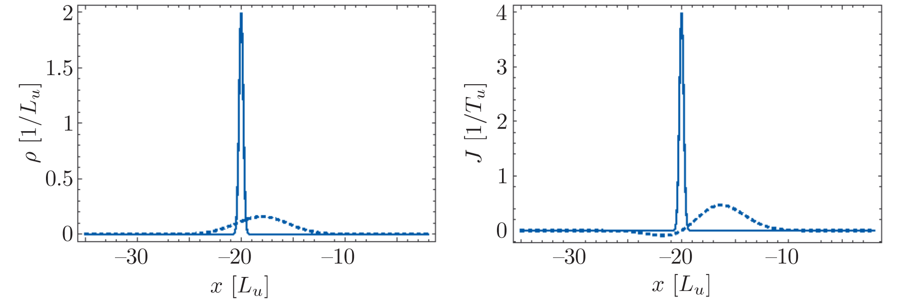

Figure 1. (a) Probability density spatial distributions emanating from an initial wave packet centred at $x_o = -20L_u$ and currying mean momentum $p = 2P_u$ at time $t = 0$ (solid curve) and at $t = 1Tu$ (dashed curve); rest of data as in common data; (b) Current spatial density at time $t = 0$ (solid curve) and at $t = 1Tu$ (dashed curve); data as in (a)

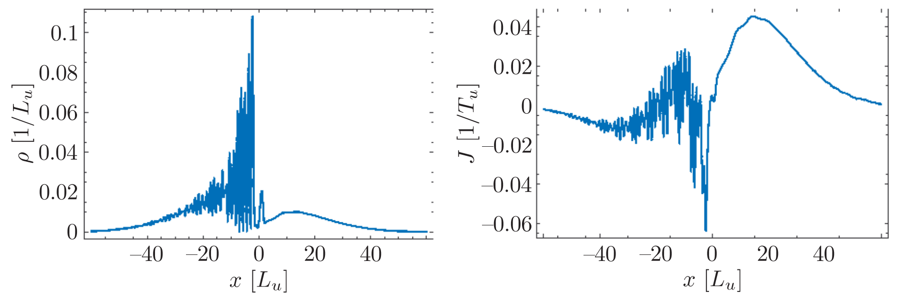

Figure 2. (a) Probability density spatial distribution at $t = 8T_u$ emanating from an initial wave packet located at $x_o = -20L_u$ and carrying a mean momentum $p = 2P_u$; rest of data as per Figure 1(a); (b) Current density spatial distribution data as per (a)

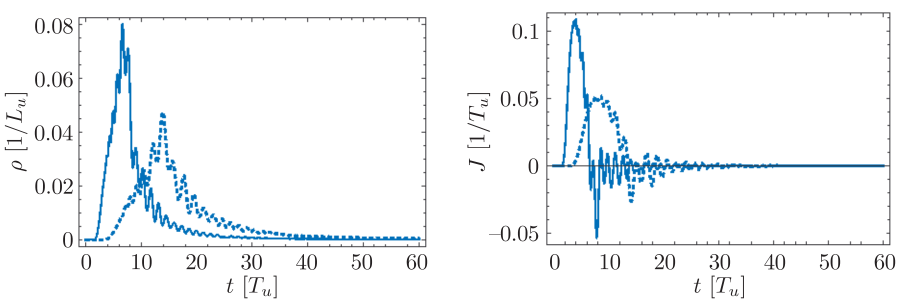

Figure 3. Probability density time evolution at the barrier entrance, $x = -a = -2L_u$, (a) resulting from initial wave packet with mean momentum $p = 2P_u$, centred at $x_o = -20L_u$ (solid curve), and at $x_o = -40L_u$ (dashed curve); rest of data those in common; (b) depicts corresponding current densities

Finally, the figure below depicts the transmission coefficient as a function of the mean momentum curried by the initial wave packet. Clearly, one notices transmission in case the mean momentum points away from the barrier.

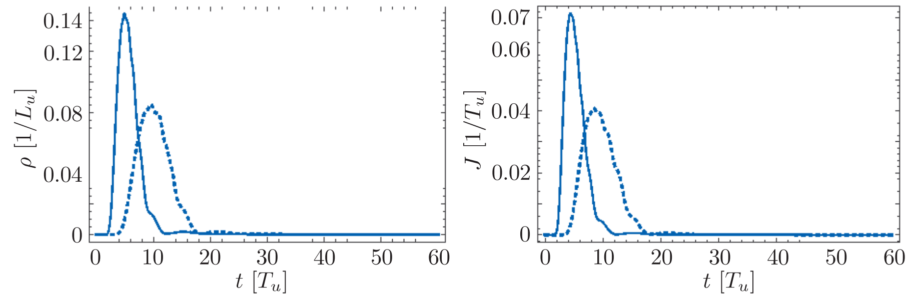

Figure 4. (a) shows probability density evolutions at the barrier exit, $x = a = 2L_u$, associated with data as per Figure 3(a); Corresponding current density time evolutions are depicted in (b)

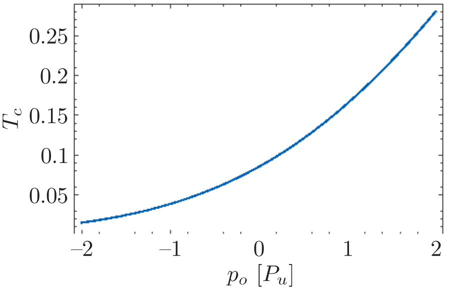

Figure 5. Transmission coefficient versus mean momentum carried by the initial wave packet located at $x_o = -20L_u$. Same result for different value of x_o in region (1) with negligible wave packet-barrier overlap; rest of data those in common

It should be noted that through pertinent calculations it is verified that the transmission coefficient does not depend on the initial wave packet location.

5. Conclusion

In conclusion we may accentuate the following points from the above study namely:

i) Independence of the transmission coefficient, for a given wave packet, of its initial location. The further away the initial location from the barrier it takes somewhat longer for transmission to be completed.

ii) The current density at the barrier entrance starts by getting into and out of the barrier repeatedly over a long time until it essentially nullifies, while at the same time exits the barrier uni-directionally. Over extremely long time the probability entering the barrier equals the one exiting the barrier. Furthermore, the transmission coefficient can be obtained either from the probability entering or exiting the barrier over an extremely long time. At such a long time the transmission coefficient can be, also, obtained from the transmitted spatial distribution.

iii) There appears probability transmission through the barrier even if the initial wave packet mean momentum points away from the barrier.

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