Exact vs. quasi-classical tunneling times for idealized potentials

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Abstract: We compare the exact tunneling time with the quasi-classical tunneling time for idealized potentials. We examine three one-dimensional cases where the potential is chosen to have a simple form. In each case, the exact tunneling time and the quasi-classical time differ significantly. In one case, the two differ in magnitude by a factor of about ten. In another case, the two differ not only quantitatively, but qualitatively as well. A discussion is given as to why the two times are significantly different, and suggestions for further inquiries are made.

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Résumé : Nous comparons les temps exact et semi-classique de la transition tunnel pour certains potentiels modèles. Nous examinons trois potentiels 1-D de forme simple. Dans tous les cas, le temps exact et le temps semi-classique diffèrent de façon significative. Dans un cas, ils diffèrent par un ordre de grandeur. Dans un autre cas, les deux diffèrent non seulement quantitativement, mais aussi qualitativement. Nous cherchons des causes possibles et suggérons des études additionnelles.

[Traduit par la Rédaction]

1. Introduction

Tunneling phenomena in quantum mechanics have been an active area of research for many years. Lately, there has been a growing interest in tunneling phenomena [1–5] primarily for two reasons. First, with increasing technological advancement, quantum-well structures can now be constructed so that tunneling can be examined experimentally [6]. Secondly, there has been some debate in the literature over which definition one should use to determine the time it takes for a particle to "tunnel" through a potential barrier (see, e.g., refs. 1 and 4). This debate arises primarily because there is no operator associated with time in quantum mechanics. This leads to an ambiguity in defining quantities that have units of time. More recently, it was shown in ref. 7 that the dwell-time definition for tunneling times, as defined in the standard or Copenhagen interpretation of quantum mechanics, agrees with the tunneling time that one would compute in the Bohmian interpretation of quantum mechanics, where it is much more straightforward and unambiguous to define the tunneling time. As we will see, this is important because our definition of tunneling times from localized states is very similar to that defined in ref. 7. It

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should be pointed out that the various definitions for tunneling times mentioned above do not hold for the case of tunneling from a localized state [1]. As interesting as this area of research is, in this paper, we will be concerned only with tunneling from localized states, and will not consider further the debate as to the proper definition for tunneling times from nonlocalized states.

In many books on quantum mechanics, the phenomenon of tunneling is discussed, and a formula is given for estimating the tunneling time (see, e.g., refs. 8–11). We will refer to this formula as the "quasi-classical" tunneling time, as it relies on quasi-classical concepts.

The basic idea underlying the formula is to think of the particle as making several attempts to tunnel through the potential barrier, and to use or estimate the probability, P, that the particle will tunnel through the barrier on a given attempt. Let Δt_{qc} denote the time interval between attempts. The average number $< N >$ of attempts taken for the particle to finally tunnel is just $< N >= 1/P$. Thus, the quasi-classical tunneling time, t_{qc}, is given by

$$t_{qc} = \Delta t_{qc} < N >= \frac{1}{P}\Delta t_{qc} \tag{1}$$

In the quasi-classical formulation, Δt_{qc} is estimated by

$$\Delta t_{qc} = \frac{2R}{v} \tag{2}$$

where R is the width of the well and v is the speed of the particle as it moves inside the well.

One could expect that t_{qc} would not agree with the exact tunneling time, t_{tun}, on the grounds that, for example, v must change with time as the wave function of the particle develops in time as described by the Schrödinger equation.

The principal objective of this paper is to calculate the tunneling time exactly for selected idealized one-dimensional cases and thereby inquire as to the degree of success resulting through the use of t_{qc} instead. One of the main reasons motivating this investigation is that the quasi-classical formula is frequently used to calculate the tunneling time, even in cases where, in our view, use of the formula is questionable. We, therefore, examine three cases, two of which have the potential barrier modeled as a simple δ-function barrier, the other being a double-square-well potential. We will show that t_{qc} is not necessarily a reliable means of estimating the tunneling time.

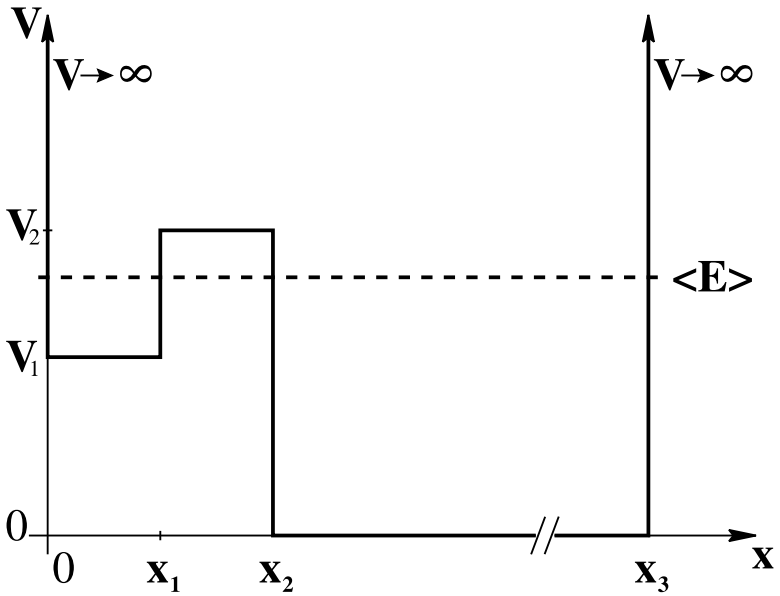
2. Delta-function potential barrier

We will consider how the tunneling time depends upon various parameters for cases where the potential energy has the ideal form shown in Fig. 1. Here we are dealing with a particle that is placed at time $t = 0$ inside the narrow, shallow well (i.e., the particle is initially localized in the range $0 < x < x_1$). We ensure that the expectation value $< E >$ of the particle's total energy is less than the barrier height V_2. We calculate exactly the time taken for the particle to tunnel out of the inner well and into the wide, deep outer well.

By taking $x_2 \to x_1^+$ and $V_2 \to \infty$, we simplify the double-well problem to that of tunneling past a δ-function potential barrier. We consider this simpler case in this section, dealing with the full double-well problem in the next section.

We, therefore, first consider a particle initially localized in the range $0 < x < x_1$, with a δ-function potential barrier located at $x = x_1$; we also confine the particle for all time to the range $0 < x < x_2$. (Note that we simply rename x_3 and refer to it as x_2 for the δ-function cases.) We first take the potential on either side of the barrier to be the same (i.e. we choose $V_1 = 0$). In the second example, we will have the potential higher inside the barrier (i.e., $V_1 > 0$), so that the problem is more truly a "tunneling problem".

Fig. 1. The potential energy of the double square well with a square potential barrier. The expectation value $< E >$ of the particle energy is such that $V_1 << E >> V_2$.



Our method for calculating the exact value of the tunneling time is as follows. First we calculate the eigenfunctions of the Hamiltonian. After choosing an initial state for the particle, we express the time-dependent wave function in terms of the eigenstates of the Hamiltonian. We then write the expression for the exact tunneling time in terms of the time-dependent wave function of the particle. At that point we must make use of a computer. Doing so gives us our desired results.

We thus take the potential to be given by

$$V(x) = \begin{cases} +\infty, & \text{for} \quad x \leq 0 \\ V_1, & \text{for} \quad 0 < x < x_1 \\ \lambda\delta(x - x_1), & \text{for} \quad x = x_1 \\ 0, & \text{for} \quad x_1 < x < x_2 \\ +\infty, & \text{for} \quad x_2 \leq x \end{cases} \tag{3}$$

The Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_k(x)}{\mathrm{d}x^2} + V(x)\psi_k(x) = E_k\psi_k(x) \tag{4}$$

allows us to determine all the energy eigenfunctions, $\psi_k(x)$, and the corresponding energy eigenvalues, $E = E_k = \hbar^2k^2/(2m)$, where m is the mass of the particle.

It is straightforward to show that the eigenfunctions have the form

$$\psi_k(x) = \begin{cases} \psi_k^{\mathrm{I}}(x), & \text{for} \quad E < V_1 \\ \psi_k^{\mathrm{II}}(x), & \text{for} \quad E > V_1 \end{cases} \tag{5}$$

$$\psi_k^{\mathrm{I}}(x) = \begin{cases} 0, & \text{for} \quad x \le 0 \\ A_1 \ \sinh(qx), & \text{for} \quad 0 < x < x_1 \\ B_1 \ \sin[k(x - x_2)], & \text{for} \quad x_1 < x < x_2 \\ 0, & \text{for} \quad x_2 \le x \end{cases} \tag{6}$$

$$\psi_k^{\mathrm{II}}(x) = \begin{cases} 0, & \text{for} \quad x \le 0 \\ A_2 \ \sin(px), & \text{for} \quad 0 < x < x_1 \\ B_2 \ \sin[k(x - x_2)], & \text{for} \quad x_1 < x < x_2 \\ 0, & \text{for} \quad x_2 \le x \end{cases} \tag{7}$$

where $k^2 = 2mE/\hbar^2$, $q^2 = 2m(V_1 - E)/\hbar^2$, $p^2 = 2m(E - V_1)/\hbar^2$.

We solve for the energies E and eigenfunctions ψ_k by imposing continuity of the eigenfunctions across the barrier, normalizing, and using the discontinuity of $\mathrm{d}\psi_k/\mathrm{d}x$ at $x = x_1$

$$\left[\frac{\mathrm{d}\psi_k(x)}{\mathrm{d}x}\right]_{x_1^+} - \left[\frac{\mathrm{d}\psi_k(x)}{\mathrm{d}x}\right]_{x_1^-} = \frac{2m\lambda}{\hbar^2}\psi_k(x_1) \tag{8}$$

The eigenvalue conditions turn out to be

$$k\cot[k(x_2 - x_1)] + q\coth(qx_1) = -\frac{2m\lambda}{\hbar^2}, \qquad \text{for} \qquad E < V_1 \tag{9}$$

$$k\cot[k(x_2 - x_1)] + p\cot(px_1) = -\frac{2m\lambda}{\hbar^2}, \qquad \text{for} \qquad E > V_1 \tag{10}$$

The coefficients A_1, A_2, B_1, and B_2 are found by continuity of the wave function at $x = x_1$, (8) for the discontinuity of $\mathrm{d}\psi_k/\mathrm{d}x$ at $x = x_1$, and by normalizing ψ_k: $\int_{-\infty}^{+\infty} |\psi_k(x)|^2 \, \mathrm{d}x = 1$. After some straightforward calculation, we obtain

$$|A_1|^{-2} = \frac{(x_2 - x_1)\sinh^2(qx_1)}{2\sin^2[k(x_2 - x_1)]} - \frac{x_1}{2} + \frac{\sinh(2qx_1)}{4q} - \frac{\sinh^2(qx_1)\cot[k(x_2 - x_1)]}{2k} \tag{11}$$

$$|A_2|^{-2} = \frac{(x_2 - x_1)\sin^2(px_1)}{2\sin^2[k(x_2 - x_1)]} + \frac{x_1}{2} - \frac{\sin(2px_1)}{4p} - \frac{\sin^2(px_1)\cot[k(x_2 - x_1)]}{2k} \tag{12}$$

The problem is simplified by choosing $(x_2 - x_1) \to \infty$; we get

$$|A_1|^2 \approx \frac{2\sin^2[k(x_2 - x_1)]}{(x_2 - x_1)\sinh^2(qx_1)} \tag{13}$$

$$|A_2|^2 \approx \frac{2\sin^2[k(x_2 - x_1)]}{(x_2 - x_1)\sin^2(px_1)} \tag{14}$$

Expressions for B_1 and B_2 are obtained in a similar manner.

We choose the initial state of the particle to be the state corresponding to the lowest energy if the potential were to be infinite for $x > x_1$; i.e., in an infinitely deep potential well. The initial state is thus given by

$$\psi_0(x) \equiv \psi(x, t = 0) = \begin{cases} \sqrt{\frac{2}{x_1}} \sin\left(\frac{\pi x}{x_1}\right), & \text{for } 0 < x < x_1 \\ 0, & \text{elsewhere} \end{cases} \tag{15}$$

We can now write the time dependence of this state by exploiting the completeness of the energy eigenstates. At $t = 0$ we have

$$\psi_0(x) = \sum_{E_k} C_k \psi_k(x) \tag{16}$$

with

$$C_k =< \psi_k|\psi_0 >= \begin{cases} C_k^{\mathrm{I}} =< \psi_k^{\mathrm{I}}|\psi_0 >, & \text{for } E < V_1 \\ C_k^{\mathrm{II}} =< \psi_k^{\mathrm{II}}|\psi_0 >, & \text{for } E > V_1 \end{cases} \tag{17}$$

Then the time-dependent wave function is given by

$$\psi(x,t) = \sum_E C_k\ \psi_k(x)\, \mathrm{e}^{-iEt/\hbar} = \sum_{E<V_1} C_k^{\mathrm{I}}\ \psi_k^{\mathrm{I}}(x)\, \mathrm{e}^{-iEt/\hbar} + \sum_{E>V_1} C_k^{\mathrm{II}}\ \psi_k^{\mathrm{II}}(x)\, \mathrm{e}^{-iEt/\hbar} \tag{18}$$

The exact tunneling time can now be calculated, because we know the wave function $\psi(x,t)$ exactly. (Note that C_k^{I} and C_k^{II} are given implicitly below in dimensionless form.) Our only limitation will be that, ultimately, we will need to make use of a computer, so the "exact" value of the tunneling time can be determined to the desired number of significant figures. We will see that this poses no problems in our quest to compare t_{qc} and the exact time t_{tun}.

As discussed in the introduction, there is much debate in the literature over which definition of the tunneling time from nonlocalized states is the correct one. In ref. 7, it was shown that the dwell-time definition agreed with that obtained from computing the tunneling time in the Bohmian interpretation of quantum mechanics, supporting this definition of the tunneling time. We define the tunneling time, t_{tun}, from a localized state (as is the case for the configurations we deal with throughout this paper) in a very similar manner to that done in ref. 7

$$t_{\mathrm{tun}} = \frac{\int_0^\infty t\, P_{\mathrm{in}}(t)\, \mathrm{d}t}{\int_0^\infty P_{\mathrm{in}}(t)\, \mathrm{d}t} \tag{19}$$

where

$$P_{\mathrm{in}}(t) = \int_0^{x_1} |\psi(x,t)|^2\, \mathrm{d}x \tag{20}$$

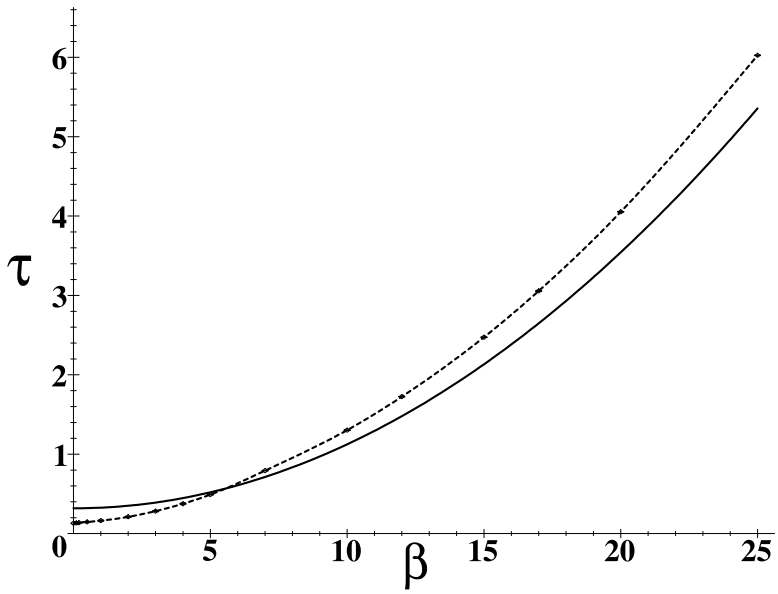
We will refer to this tunneling time as "the exact tunneling time".

From the eigenvalue conditions, (9) and (10), one can deduce that the difference Δk between consecutive eigenvalues is, in the limit $(x_2 - x_1) \to \infty$, $\Delta k \approx \pi/(x_2 - x_1)$. Moreover, in the limit $(x_2 - x_1) \to \infty$, one can replace the sum by an integral. Since we will soon need to make use of a computer to calculate t_{tun}, we convert $\psi(x,t)$ to dimensionless form, as follows:

$$\phi(\eta,\tau) = \begin{cases} \phi_1(\eta,\tau), & \text{for} \quad 0 < \eta < 1 \\ \phi_2(\eta,\tau), & \text{for} \quad 1 < \eta < \eta_1 \equiv x_2/x_1 \\ 0, & \text{elsewhere} \end{cases} \tag{21}$$

$$\phi_1(\eta,\tau) = 2\sqrt{2} \int_0^{\kappa_1} \mathrm{d}\kappa \frac{\kappa^2 \sinh(\mu) \sinh(\mu\eta)\, \mathrm{e}^{-i\kappa^2\tau}}{(\pi^2+\mu^2)\left\{\kappa^2 \sinh^2(\mu) + f^2(\kappa,\beta)\right\}} + 2\sqrt{2} \int_{\kappa_1}^{\infty} \mathrm{d}\kappa \frac{\kappa^2 \sin(\rho) \sin(\rho\eta)\, \mathrm{e}^{-i\kappa^2\tau}}{(\pi^2-\rho^2)\left\{\kappa^2 \sin^2(\rho) + g^2(\kappa,\beta)\right\}} \tag{22}$$

Fig. 2. The quasi-classical tunneling time τ_{qc} (continuous-line curve) and the exact tunneling time τ_{tun} (broken-line curve) as a function of the strength β of the δ-function potential for the case $\upsilon_1 = 0$.



$$\phi_2(\eta,\tau) = 2\sqrt{2}\int_0^{\kappa_1} \mathrm{d}\kappa \frac{\kappa \sinh(\mu)\ \{\kappa \sinh(\mu)\cos[\kappa(\eta-1)] + f(\kappa,\beta)\sin[\kappa(\eta-1)]\}\ \mathrm{e}^{-i\kappa^2\tau}}{(\pi^2+\mu^2)\left\{\kappa^2\sinh^2(\mu) + f^2(\kappa,\beta)\right\}}$$
$$+ 2\sqrt{2}\int_{\kappa_1}^{\infty} \mathrm{d}\kappa \frac{\kappa \sin(\rho)\ \{\kappa \sin(\rho)\cos[\kappa(\eta-1)] + g(\kappa,\beta)\sin[\kappa(\eta-1)]\}\ \mathrm{e}^{-i\kappa^2\tau}}{(\pi^2-\rho^2)\left\{\kappa^2\sin^2(\rho) + g^2(\kappa,\beta)\right\}} \quad (23)$$

with

$$f(\kappa,\beta) = \beta\sinh(\mu) + \mu\cosh(\mu) \quad (24)$$

$$g(\kappa,\beta) = \beta\sin(\rho) + \rho\cos(\rho) \quad (25)$$

where we have defined the following dimensionless quantities: $\phi = \sqrt{x_1}\psi$, $\kappa = kx_1$, $\mu = qx_1$, $\rho = px_1$, $\kappa_1 = x_1\sqrt{2mV_1}/\hbar$, $\beta = 2mx_1\lambda/\hbar^2$, $\eta = x/x_1$, $\tau = t/t_0$, and $t_0 = 2mx_1^2/\hbar$.

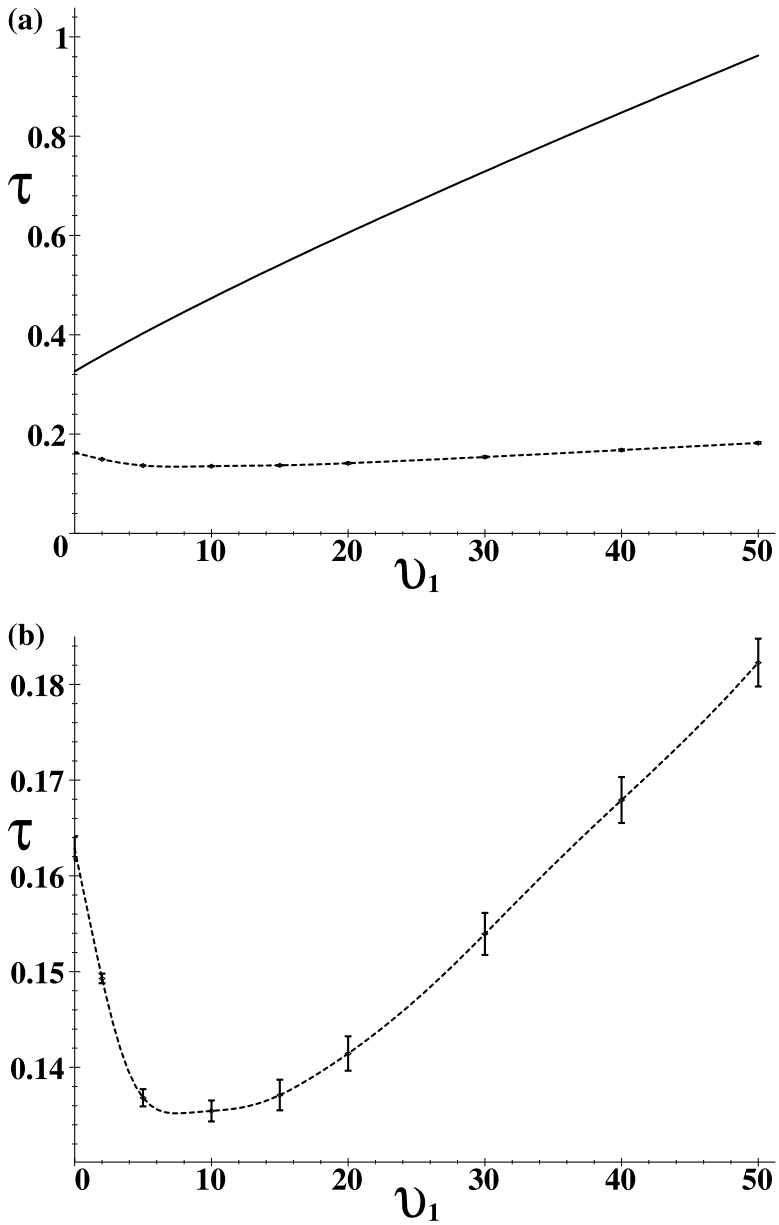
We should note at this point that our results in (22) and (23) agree with what was done in ref. 12. In ref. 12, tunneling through a delta-function barrier was examined, where the potential used was identical to ours if one puts $V_1 = 0$ in (3) of our paper. If we reduce our more general equations, by setting $V_1 = 0$, we reproduce exactly eq. (1) of ref. 12.

Next we recall the method used to calculate the quasi-classical tunneling time. Typically, one begins by calculating the probabilities of reflection and of transmission for a particle incident on the barrier "from the left" and with flux $\hbar k/m$. One thus calculates the reflection coefficient, R, and the transmission coefficient, T, in the standard manner. The quasi-classical tunneling time is then given by (1) with $P = |T|^2$.

The quasi-classical tunneling time can be expressed in dimensionless units as follows:

$$P = |T|^2 = \left|\frac{(2\rho)}{(\kappa+\rho+i\beta)}\right|^2, \qquad \tau_{qc} = \frac{1}{\pi\ |T|^2} = \frac{(\kappa+\rho)^2+\beta^2}{4\pi\rho^2} \quad (26)$$

Fig. 3. The quasi-classical tunneling time τ_{qc} (continuous-line curve) and the exact tunneling time τ_{tun} (broken-line curve) as a function of υ_1 for a δ-function potential with $\beta = 1$. Note that τ_{qc} is incorrect both quantitatively and qualitatively. In part (b), τ_{tun} is shown alone so that its qualitative features are clearly seen.



In Figs. 2 and 3, we compare the exact tunneling time τ_{tun} and the quasi-classical tunneling time τ_{qc}. In Fig. 2, we show how they depend on the dimensionless strength of the δ-function potential barrier. Though they both have the same qualitative behaviour, they do not have the same value. The difference is not alarming, even though it is noteworthy.

In Figs. 3*a* and 3*b*, we show τ_{qc} and τ_{tun} for a fixed strength of the barrier, but with the value of $\upsilon_1 \equiv 2mx_1^2 V_1/\hbar^2$ increasing. Figures 3*a* and 3*b* show that the two are significantly different: not only

does τ_{qc} have the wrong value, it also fails to reveal the correct qualitative trend.

We will discuss this further after we deal with the double-square-well case.

3. Square potential barrier

We next consider the full double-well potential shown explicitly in Fig. 1. The potential is given by

$$V(x) = \begin{cases} +\infty, & \text{for} \quad x \le 0 \\ V_1, & \text{for} \quad 0 < x < x_1 \\ V_2, & \text{for} \quad x_1 < x < x_2 \\ 0, & \text{for} \quad x_2 < x < x_3 \\ \infty, & \text{for} \quad x_3 \le x \end{cases} \tag{27}$$

The Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_k(x)}{\mathrm{d}x^2} + V(x)\psi_k(x) = E_k\psi_k(x) \tag{28}$$

The eigenfunctions have the form

$$\psi_k(x) = \begin{cases} \psi_k^{\mathrm{I}}(x), & \text{for} \quad E < V_1 \\ \psi_k^{\mathrm{II}}(x), & \text{for} \quad V_1 < E < V_2 \\ \psi_k^{\mathrm{III}}(x), & \text{for} \quad V_2 < E \end{cases} \tag{29}$$

where

$$\psi_k^{\mathrm{I}}(x) = \begin{cases} A_1\,\mathrm{e}^{q_1 x} + B_1\,\mathrm{e}^{-q_1 x}, & \text{for} \quad 0 < x < x_1 \\ C_1\,\mathrm{e}^{q_2 x} + D_1\,\mathrm{e}^{-q_2 x}, & \text{for} \quad x_1 < x < x_2 \\ E_1\,\mathrm{e}^{ikx} + F_1\,\mathrm{e}^{-ikx}, & \text{for} \quad x_2 < x < x_3 \\ 0, & \text{elsewhere} \end{cases} \tag{30}$$

$$\psi_k^{\mathrm{II}}(x) = \begin{cases} A_2\,\mathrm{e}^{ip_1 x} + B_2\,\mathrm{e}^{-ip_1 x}, & \text{for} \quad 0 < x < x_1 \\ C_2\,\mathrm{e}^{q_2 x} + D_2\,\mathrm{e}^{-q_2 x}, & \text{for} \quad x_1 < x < x_2 \\ E_2\,\mathrm{e}^{ikx} + F_2\,\mathrm{e}^{-ikx}, & \text{for} \quad x_2 < x < x_3 \\ 0, & \text{elsewhere} \end{cases} \tag{31}$$

and

$$\psi_k^{\mathrm{III}}(x) = \begin{cases} A_3\,\mathrm{e}^{ip_1 x} + B_3\,\mathrm{e}^{-ip_1 x}, & \text{for} \quad 0 < x < x_1 \\ C_3\,\mathrm{e}^{ip_2 x} + D_3\,\mathrm{e}^{-ip_2 x}, & \text{for} \quad x_1 < x < x_2 \\ E_3\,\mathrm{e}^{ikx} + F_3\,\mathrm{e}^{-ikx}, & \text{for} \quad x_2 < x < x_3 \\ 0, & \text{elsewhere} \end{cases} \tag{32}$$

We have defined $k^2 = 2mE/\hbar^2$, $q_i^2 = 2m(V_i - E)/\hbar^2$, and $p_i^2 = 2m(E - V_i)/\hbar^2$.

The initial state is again given by

$$\psi_0(x) \equiv \psi(x, t = 0) = \begin{cases} \sqrt{\frac{2}{x_1}}\sin\left(\frac{\pi x}{x_1}\right), & \text{for} \quad 0 < x < x_1 \\ 0, & \text{elsewhere} \end{cases} \tag{33}$$

Then, proceeding as before

$$\psi_0(x) = \sum_{E_k} C_k \ \psi_k(x)$$

with

$$C_k =< \psi_k|\psi_0 >= \begin{cases} C_k^{\rm I} =< \psi_k^{\rm I}|\psi_0 >, & \text{for} \quad E < V_1 \\ C_k^{\rm II} =< \psi_k^{\rm II}|\psi_0 >, & \text{for} \quad V_1 < E < V_2 \\ C_k^{\rm III} =< \psi_k^{\rm III}|\psi_0 >, & \text{for} \quad V_2 < E \end{cases} \tag{34}$$

The initial state, expressed in terms of energy eigenfunctions (in dimensionless units), is

$$\psi_0(\eta) = \sum_{E<V_1} C_k^{\rm I}\psi_0^{\rm I}(\eta,\kappa) + \sum_{V_1<E<V_2} C_k^{\rm II}\psi_0^{\rm II}(\eta,\kappa) + \sum_{E>V_2} C_k^{\rm III}\psi_0^{\rm III}(\eta,\kappa) \tag{35}$$

with

$$\psi_0^{\rm I}(\eta,\kappa) = \begin{cases} \sinh(\mu_1\eta), & \text{for} \quad 0 < \eta < \eta_1 \\ \sinh(\mu_1\eta_1)\cosh[\mu_2(\eta-\eta_1)] & \\ \qquad +\frac{\mu_1}{\mu_2}\cosh(\mu_1\eta_1)\sinh[\mu_2(\eta-\eta_1)], & \text{for} \quad \eta_1 < \eta < \eta_2 \\ \frac{\sin[\kappa(\eta_3-\eta)]}{\sin[\kappa(\eta_3-\eta_2)]}(\sinh(\mu_1\eta_1)\cosh[\mu_2(\eta_2-\eta_1)] & \\ \qquad +\frac{\mu_1}{\mu_2}\cosh(\mu_1\eta_1)\sinh[\mu_2(\eta_2-\eta_1)]), & \text{for} \quad \eta_2 < \eta < \eta_3 \\ 0, & \text{elsewhere} \end{cases} \tag{36}$$

$$\psi_0^{\rm II}(\eta,\kappa) = \begin{cases} \sin(\rho_1\eta), & \text{for} \quad 0 < \eta < \eta_1 \\ \sin(\rho_1\eta_1)\cosh[\mu_2(\eta-\eta_1)] & \\ \qquad +\frac{\rho_1}{\mu_2}\cos(\rho_1\eta_1)\sinh[\mu_2(\eta-\eta_1)], & \text{for} \quad \eta_1 < \eta < \eta_2 \\ \frac{\sin[\kappa(\eta_3-\eta)]}{\sin[\kappa(\eta_3-\eta_2)]}(\sin(\rho_1\eta_1)\cosh[\mu_2(\eta_2-\eta_1)] & \\ \qquad +\frac{\rho_1}{\mu_2}\cos(\rho_1\eta_1)\sinh[\mu_2(\eta_2-\eta_1)]), & \text{for} \quad \eta_2 < \eta < \eta_3 \\ 0, & \text{elsewhere} \end{cases} \tag{37}$$

and

$$\psi_0^{\rm III}(\eta,\kappa) = \begin{cases} \sin(\rho_1\eta), & \text{for} \quad 0 < \eta < \eta_1 \\ \sin(\rho_1\eta_1)\cos[\rho_2(\eta-\eta_1)] & \\ \qquad +\frac{\rho_1}{\rho_2}\cos(\rho_1\eta_1)\sin[\rho_2(\eta-\eta_1)], & \text{for} \quad \eta_1 < \eta < \eta_2 \\ \frac{\sin[\kappa(\eta_3-\eta)]}{\sin[\kappa(\eta_3-\eta_2)]}(\sin(\rho_1\eta_1)\cos[\rho_2(\eta_2-\eta_1)] & \\ \qquad +\frac{\rho_1}{\rho_2}\cos(\rho_1\eta_1)\sin[\rho_2(\eta_2-\eta_1)]), & \text{for} \quad \eta_2 < \eta < \eta_3 \\ 0, & \text{elsewhere} \end{cases} \tag{38}$$

Then the time-dependent wave function is given by

$$\begin{aligned} \psi(x,t) &= \sum_E C_k \ \psi_k(x)\,{\rm e}^{-iEt/\hbar} \\ &= \sum_{E<V_1} C_k^{\rm I} \ \psi_k^{\rm I}(x)\,{\rm e}^{-iEt/\hbar} + \sum_{V_1<E<V_2} C_k^{\rm II} \ \psi_k^{\rm II}(x)\,{\rm e}^{-iEt/\hbar} + \sum_{E>V_2} C_k^{\rm III} \ \psi_k^{\rm III}(x)\,{\rm e}^{-iEt/\hbar} \end{aligned} \tag{39}$$

Again, taking the limit $(\eta_3 - \eta_2) \to \infty$ allows us to replace the sum by an integral; after a lengthy calculation, $\psi(x,t)$ in dimensionless form is

$$\phi(\eta,\tau) = \begin{cases} \phi_1(\eta,\tau), & \text{for} \quad 0 < \eta < \eta_1 \\ \phi_2(\eta,\tau), & \text{for} \quad \eta_1 < \eta < \eta_2 \\ \phi_3(\eta,\tau), & \text{for} \quad \eta_2 < \eta < \eta_3 \\ 0, & \text{elsewhere} \end{cases} \tag{40}$$

$$\begin{aligned} \phi(\eta,\tau) = 2\sqrt{2}\int_0^{\kappa_1} \mathrm{d}\kappa \, & \frac{\mu_2^2 \sinh(\mu_1\eta_1)\psi_0^{\mathrm{I}}(\eta,\kappa)\left[1+T_1^{-2}(\kappa)\right]^{-1} \mathrm{e}^{-i\kappa^2\tau}}{\left(\mu_1^2+\pi^2\right)\left[\mu_2\sinh(\mu_1)\cosh(\mu_2 N)+\mu_1\cosh(\mu_1)\sinh(\mu_2 N)\right]^2} \\ + 2\sqrt{2}\int_{\kappa_1}^{\kappa_2} \mathrm{d}\kappa \, & \frac{\mu_2^2 \sin(\rho_1\eta_1)\psi_0^{\mathrm{II}}(\eta,\kappa)\left[1+T_2^{-2}(\kappa)\right]^{-1} \mathrm{e}^{-i\kappa^2\tau}}{\left(\mu_1^2+\pi^2\right)\left[\mu_2\sin(\rho_1)\cosh(\mu_2 N)+\rho_1\cos(\rho_1)\sinh(\mu_2 N)\right]^2} \\ + 2\sqrt{2}\int_{\kappa_2}^{\infty} \mathrm{d}\kappa \, & \frac{\rho_2^2 \sin(\rho_1\eta_1)\psi_0^{\mathrm{III}}(\eta,\kappa)\left[1+T_3^{-2}(\kappa)\right]^{-1} \mathrm{e}^{-i\kappa^2\tau}}{\left(\mu_1^2+\pi^2\right)\left[\rho_2\sin(\rho_1)\cos(\rho_2 N)+\rho_1\cos(\rho_1)\sin(\rho_2 N)\right]^2} \end{aligned} \tag{41}$$

with

$$T_1 = \frac{-\kappa}{\mu_2}\left[\frac{\mu_2\tanh(\mu_1\eta_1)+\mu_1\tanh(\mu_2 N)}{\mu_2\tanh(\mu_1\eta_1)\tanh(\mu_2 N)+\mu_1}\right] \tag{42}$$

$$T_2 = \frac{-\kappa}{\mu_2}\left[\frac{\mu_2\tan(\rho_1\eta_1)+\rho_1\tanh(\mu_2 N)}{\mu_2\tan(\rho_1\eta_1)\tanh(\mu_2 N)+\rho_1}\right] \tag{43}$$

$$T_3 = \frac{\kappa}{\rho_2}\left[\frac{\rho_2\tan(\rho_1\eta_1)+\rho_1\tan(\rho_2 N)}{\rho_2\tan(\rho_1\eta_1)\tan(\rho_2 N)-\rho_1}\right] \tag{44}$$

where we have defined the following dimensionless quantities: $\phi = \sqrt{x_1}\psi$, $\eta = x/x_1$, $\eta_i = x_i/x_1$, $N = \eta_2 - \eta_1$, $\kappa = kx_1$, $\kappa_i = x_1\sqrt{2mV_i}/\hbar$, $\mu_i = \sqrt{\kappa_i^2 - \kappa^2}$, $\rho_i = \sqrt{\kappa^2 - \kappa_i^2}$, $\tau = t/t_0 = \hbar t/(2mx_1^2)$, with $t_0 = 2mx_1^2/\hbar$.

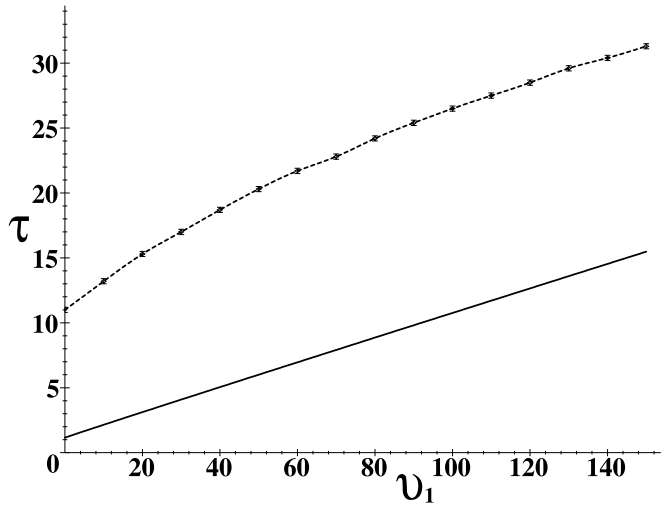
In Fig. 4, we compare the quasi-classical tunneling time, τ_{qc}, with the exact tunneling time, τ_{tun}. In this figure, the energies are again given in units of $\hbar^2/(2mx_1^2)$; i.e., $\upsilon_1 \equiv 2mx_1^2V_1/\hbar^2$, $\upsilon_2 \equiv 2mx_1^2V_2/\hbar^2$, and $\epsilon \equiv 2mx_1^2E/\hbar^2$. The two differ by a factor of up to about ten. Even though τ_{qc} has the right qualitative behaviour, it is as much as an order of magnitude too large.

4. Numerical methods

The numerical computation of the wave function is not trivial; we thus briefly describe the key features of the methods that we used.

Equation (20) was evaluated for a series of τ values. The integrals in (20), (22), and (41) were computed using Simpson's rule. The integral over wave number was truncated at a sufficiently high value to allow for convergence. Since the integrand contains terms of the form $\exp(-i\kappa^2\tau)$, these terms oscillate rapidly in the time domain. To deal with the rapid oscillations, the value of κ used to truncate the integral was in turn used to compute an appropriate time step required in employing Simpson's rule for the numerical integration, allowing the numerical routine to yeild accurate results for even the most rapid oscillations in the integrand. Then the tunneling time, (19), was obtained in two

Fig. 4. The quasi-classical tunneling time τ_{qc} (continuous-line curve) and the exact tunneling time τ_{tun} (broken-line curve) for the double square well of Fig. 1. Note that τ_{qc} is a factor of up to about ten times too large. The tunneling times are plotted for increasing υ_1 but with $\upsilon_2 - \upsilon_1$ and $< \epsilon > \ - \upsilon_1$ fixed. In this figure, $\upsilon_2 - \upsilon_1 = 10$ and $< \epsilon > \ - \upsilon_1 = \pi^2$.



ways: splines and interpolation. The data points obtained from (20) were used to create a spline, which could be integrated analytically. Since the tunneling time is a ratio of two integrals containing $P_{\text{in}}(t)$, it converges for sufficiently large τ. To confirm the value obtained by the spline method and also to estimate an error for the tunneling time, we interpolated the data points from (20) with a function of the form $P'(\tau) = [\cos(a\tau + b) + 1] \exp c\tau + d$. Inserting this function into (19), we were then able to evaluate the tunneling time, (19), analytically. The tunneling times for the square potential barrier were obtained in a similar fashion.

5. Discussion

Some of the results we have found are strongly counterintuitive, which is not necessarily surprising, as this is quite common in quantum mechanics. Nevertheless, we report that we tested our results in numerous ways to ensure they are correct. As just one example, we wrote two separate programs, one for the δ-function cases, one for the double-square-well case. We compared them by letting $V_2 \to V_1^+$ for the latter, and then rescaled, such that the range $0 < x < x_2$ for the latter coincided with the range $0 < x < x_1$ of the former. Taking $\lambda = 0$ for the δ-function case, and starting with the same initial wave function for both cases, we found that both programs gave exactly the same time evolution of the initial wave function. We performed several other tests to ensure that the results reported here are correct.

One of the more interesting features of the behaviour of the tunneling time, t_{tun}, reported here is that t_{tun} increases monotonically with V_1 for the double well. One might have expected that it would decrease with V_1. Similarly, the behaviour found in Fig. 3*b* is perhaps not what one might have expected before carrying out the calculation.

There has been a great deal of discussion in the literature on resonant tunneling phenomenon. This is primarily because the process can now be demonstrated experimentally [6]. As discussed in ref. 13, when one has a double-well structure, and investigates tunneling behaviour in the system for various potential strengths, one will find resonant conditions for tunneling to occur. This is most easily observed in systems for which the width of the potential is the same on both sides of a barrier, or very close to one another. We did not observe any resonances in the tunneling times out of our potentials, as in our case we investigated tunneling to a semi-infinite second well. In this case, one does not expect

resonant tunneling; one would expect the particle to tunnel through the barrier always, given enough time. Resonant tunneling is an interesting phenomenon; however, it is beyond the scope of this paper.

6. Summary and outlook

That the two tunneling times can differ by an order of magnitude, and can give different qualitative trends, raises a legitimate concern about the use of the quasi-classical formula. We stated at the beginning of the paper that one could expect some difference between τ_{qc} and τ_{tun}; in the three simple examples we have studied, we have seen that there is reason to question the limits of validity of the use of τ_{qc}.

We believe that further study of this issue is warranted. Will the quasi-classical approach work reasonably if the potential is smooth, with no sharp discontinuities? Is the difference we have found between τ_{qc} and τ_{tun} due to sharp discontinuities? Our view is that it is not, but we cannot be sure until an investigation is carried out using a smooth potential, and perhaps also involving the well-known WKB approximation (see, for example, ref. 8, pp. 81–82) for $|T|^2$.

Given the results of our investigation, upon reflecting that many textbooks assign problems to the student to calculate the tunneling time using the quasi-classical, WKB equation, it seems to us that this question is an important one.

We have certainly shown that τ_{qc} is not correct in the simple cases we have examined. Indeed, this is what we expected to find. Certainly it is much easier to use τ_{qc} than to calculate τ_{tun} exactly. But, if the result for τ_{qc} is neither qualitatively nor quantitatively reliable, it is not appropriate.

We hope that this initial conceptual investigation will lead to further endeavours along these lines. We have begun an inquiry using a smooth potential.

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