Phase-Space Approach to the Tunnel Effect: A New Semiclassical Traversal Time

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We determine the semiclassical coherent-state propagator for a particle going through one-dimensional evolution in a simple barrier potential. The described semiclassical method makes use of complex trajectories which, by its turn, enables the definition of (real) traversal times in the complexified phase space. We then discuss the behavior of this time for a wave packet whose average energy is below the barrier height. [S0031-9007(97)04310-X]

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One of the most interesting questions [1] in general physics concerns the amount of time a particle spends during its movement through a potential barrier. The subject has been considered controversial given the variety of methods and alternative approaches trying to give an answer to that question. In fact the very meaning of it is debatable [2], since the notion of trajectory is devoid of meaning in quantum mechanics or, if it makes any sense, it bears no resemblance to the classical one to which the concept of time is so intimately attached.

Theoretical proposals of tunneling times can be obtained by using path integral methods which constitute one of the possible approaches. In general it is based on some kind of extension to the quantum domain of the classical relation,

$$\Delta_\Omega = \int_{t_i}^{t_f} dt \int_\Omega \delta[x - \bar{x}(t)] dx \,, \tag{1}$$

in which the transition time Δ_Ω is the time that a particle, moving according to the path $\bar{x}(t)$, spends in the space region Ω from t_i to t_f. This relation, if applied in the form of a functional, leads to some interesting results [3], but the appearance of imaginary times complicates its physical interpretation. We also remark that alternative views of quantum mechanics [2,4] seemingly provide a direct treatment to the question, being also based on the notion of trajectory.

The semiclassical method described here [5,6] is based on the stationary approximation of the coherent-state propagator,

$$K(z'', z', T) = \langle z'' | e^{-\iota \hat{H} T/\hbar} | z' \rangle \,, \tag{2}$$

where $\hat{H}$ is the Hamiltonian operator and T is the total evolution time between the harmonic oscillator coherent states labeled by

$$z'' = \frac{1}{\sqrt{2}}\left(\frac{q''}{b} + \iota\, \frac{p''}{c}\right), \qquad z' = \frac{1}{\sqrt{2}}\left(\frac{q'}{b} + \iota\, \frac{p'}{c}\right), \tag{3}$$

where b and c are, respectively, the position and momentum uncertainties conveniently chosen so that $bc = \hbar$. The dynamics generated by the present semiclassical approximation also depends on these parameters [7].

The stationary phase approximation of (2) results in a new classical dynamics governed by Hamilton-like equations

$$\iota\hbar\dot{u} = \frac{\partial \tilde{H}}{\partial v}, \qquad \iota\hbar\dot{v} = -\frac{\partial \tilde{H}}{\partial u}\,, \tag{4}$$

where

$$u = \frac{1}{\sqrt{2}}\left(\frac{q}{b} + \iota\, \frac{p}{c}\right), \qquad v = \frac{1}{\sqrt{2}}\left(\frac{q}{b} - \iota\, \frac{p}{c}\right), \tag{5}$$

and $\tilde{H} = \langle z | \hat{H} | z \rangle$. The solutions of (4) contributing to (2) satisfy $u(0) \equiv u' = z'$ and $v(T) \equiv v'' = z^{*\prime\prime}$, while $v(0) = v'$ and $u(T) = u''$ are defined by the dynamics [8]. These correspond to stationary trajectories existing in a complex phase space, where position and momentum are complex valued quantities. The approximated propagator $\tilde{K}$ is written in the form

$$\tilde{K} = \sum_{\text{all paths}} \sqrt{\mathcal{A}} \exp\left[\frac{\iota}{\hbar} S + \frac{\iota}{2\hbar} \mathcal{I} + \frac{\pi}{4}\sigma\right], \tag{6}$$

where

$$\mathcal{A} = \frac{1}{\hbar} \left| \frac{\partial^2 S}{\partial u' \partial v''} \right| \exp[-|z'|^2 - |z''|^2], \tag{7}$$

$$S = \int_0^T dt \left[\frac{\iota\hbar}{2}(v\dot{u} - \dot{v}u) - \tilde{H}\right] - \frac{\iota\hbar}{2}(v''u'' + v'u') \,, \tag{8}$$

$$\mathcal{I} = \int_0^T \frac{\partial^2 \tilde{H}}{\partial u \partial v}\, dt \,, \tag{9}$$

and σ accounts for the phases of $\mathcal{A}$. The term S is the complex action, the quantity $\mathcal{I}$ contains $\hbar$ corrections and it is necessary to correctly treat low energy states [7]. In Eq. (6) all complex trajectories satisfying the same boundary conditions (3) must be included. The validity of (6) hinges upon the value of $\hbar$. Ideally the approximation is thoroughly valid in the classical limit, that is, if $\hbar \to 0$. It is indeed exact for certain simple systems (quadratic Hamiltonians) and accurate for others [8]. The problem here is to know whether complex trajectories can also be used as useful and accurate tools in determining tunneling amplitudes.

For this task, we apply the method to calculate the semiclassical time evolution of an initially coherent wave packet launched against a simple barrier of height $V_0 = 10.0$ and width $a = 4.0$ located between $-a/2$ and $a/2$. Writing explicitly $q = x_1 + \iota p_2$ and $p = p_1 + \iota x_2$ and using the analyticity of the smoothed $\tilde{H}$, Eqs. (4) become equivalent to Hamilton's equations for x_1, p_2, p_1, and x_2 [8] governed by the real part of $\tilde{H}$. In the present case, the dynamics generated by (4) are those of a particle governed by the Hamiltonian

$$\mathrm{Re}[\tilde{H}] = \tfrac{1}{2}p_1^2 - \tfrac{1}{2}x_2^2 + \mathrm{Re}[\tilde{V}(x_1, p_2)], \qquad (10)$$

where

$$\mathrm{Re}[\tilde{V}(q)] = \pi^{-1/4} b^{-1/2} \int_{-\infty}^{\infty} e^{-(x-q)^2/b^2} V(x)\, dx, \quad (11)$$

and Re stands for the real part. This is the complexified smoothed version of the barrier potential. Notice that $\mathrm{Re}[\tilde{V}(x_1, p_2 = 0)]$ represents a broader but lower potential barrier.

If we fix z', the map in z of $|K(z, z', T)|^2$ gives phase-space information about the evolved system. The exact calculation of $K(z, z', T)$ using barrier eigenstates $\Psi_k(x)$ [9] provides elements of comparison with the semiclassical version. The exact propagator is given by

$$K(z, z', T) = \int_{-\infty}^{\infty} C_{k,z'}^{*} C_{k,z} e^{-\iota E_k T/\hbar}\, dk, \qquad (12)$$

where

$$C_{k,z} = \int_{-\infty}^{\infty} \Psi_k(x) \langle z \,|\, x \rangle\, dx, \qquad E_k = \frac{\hbar^2 k^2}{2}, \qquad (13)$$

and

$$\langle x \,|\, z \rangle = \frac{e^{-\iota pq/2\hbar}}{\sqrt{\pi^{1/2} b}} \exp\left[-\frac{(x - q)^2}{2b^2} + \iota \frac{px}{\hbar} \right]. \qquad (14)$$

Figure 1 shows two complex trajectories in the x_1-p_2 plane together with the equipotential lines of $\mathrm{Re}[\tilde{V}(x_1, p_2)]$ for a wave packet whose initial average energy $\langle E \rangle = p^2/2 < V_0$. Both trajectories connect phase-space points for which $q' = -7.0$, $p' = 4.0$, $q'' = 7.0$, $b = 1.0$, $c = 1.0$, and $T = 3.7$. The final momenta are, however, different. The trajectory labeled by $p'' = 5.0$ gives the largest contribution to the propagator amplitude at $T = 3.7$ as shown later. Such trajectory lies completely outside the real plane (the line $p_2 = 0$). In Fig. 2 contour plot maps of $|K(z'', z', T)|^2$ for a propagated coherent state with $q' = -7.0$, $p' = 4.0$, $b = 1.0$, and $c = 1.0$ are shown at the time $T = 3.6$. The semiclassical result (6) is shown in (a) and the exact one (12) in (b). There is a remarkable agreement of the semiclassical calculation with the exact one. For each point in phase space in the case (b), a complex trajectory was determined and its contribution in the propagator was calculated. As T increases, the probability distribution moves to the right. For $T = 3.6$, the maximum probability corresponds to the point $q'' \simeq 6.5$ and $p'' \simeq 5.0$. At $T = 3.7$, the maximum is approximately at $q'' = 7.0$, the point for which the stationary trajectory is shown in Fig. 1. As one can see, in this case ($p' < \sqrt{2V_0}$), the maximum is given by a complex trajectory. If the initial momentum were increased, the corresponding most contributing complex trajectory would approximate the real one. In the limit $p' \to \infty$, the initial packet would be free and the approximation exact (quadratic Hamiltonian). One also notes that the final maximum is such that $\langle p'' \rangle > \langle p' \rangle$ which corresponds to the already known phenomenon [10] of barrier induced acceleration. The barrier acts like a filter through which high energy components are preferably passed.

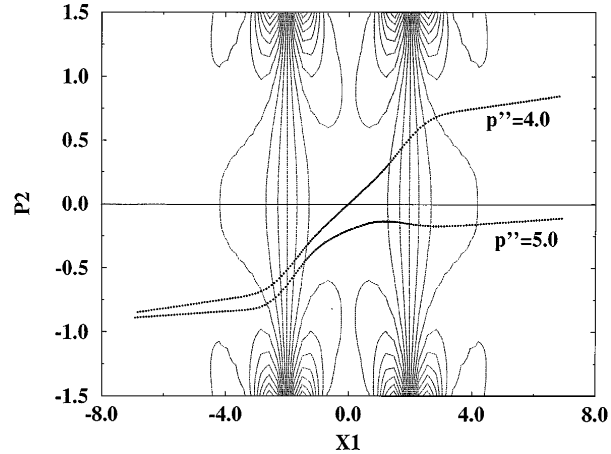

FIG. 1. Equipotential lines of $\mathrm{Re}[\tilde{V}(x_1, p_2)]$ and complex trajectories with $q' = -7.0$, $p' = 4.0$, $q'' = 7.0$, and $T = 3.6$ for different final momenta ($V_0 = 10.0$ and $a = 4.0$).

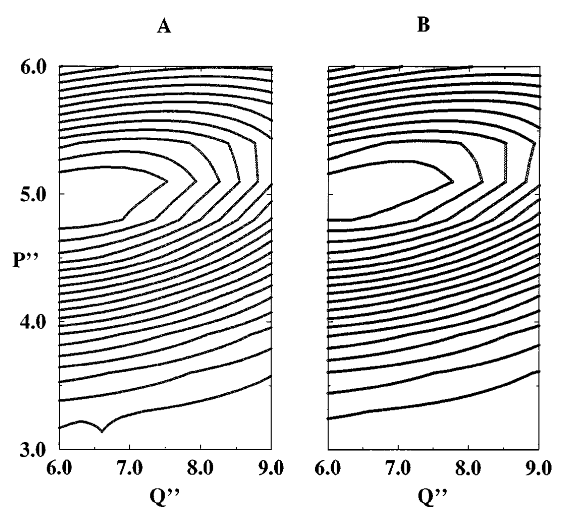

FIG. 2. Isoprobability curves of $|K(z'', z', T)|^2$ in the z'' space for an initial state with $q' = -7.0$, $p' = 4.0$, $b = 1.0$, and $c = 1.0$ at $T = 3.6$. (a) Semiclassical calculation, (b) exact calculation ($V_0 = 10.0$ and $a = 4.0$). The level curves go from zero to one at steps of 0.05.

Having thus established the accuracy of the semiclassical method, we can proceed to the determination of traversal times as defined by complex trajectories. Resorting to Eq. (1), we extend the definition of traversal times to the complex space and define, for any practical purposes, the region Ω given by $|x_1| < a/2$ as the potential limits in the x_1-p_2 plane. It is straightforward to calculate for a given trajectory the time $\Delta_\Omega(z'', z', T)$, which is the difference between the entrance and exit times in the defined Ω region for that trajectory. In the examples of Fig. 1, the trajectory labeled by $p'' = 4.0$ has $\Delta_\Omega = 1.673$, while the one for $p'' = 5.0$ has $\Delta_\Omega = 1.654$. If we admit a free movement from $q'' = -7.0$ to $q = -2.0$ with $p' = 4.0$ and from $q = 2.0$ to $q'' = 7.0$ with $p'' = 5.0$, the total time gives $t \approx 2.25$, the difference of which with respect to $T = 3.7$ is $\Delta \approx 1.45$. This value approximates very well the same value of 1.65 obtained by complex trajectories. So it is clear that, as well as the movement in phase space described by $K(z'', z', T)$ is concerned, there is a delay of the transmitted packet together with an increase of the average final momentum. More information about Δ_Ω is obtained if we introduce averages. The most probable time for the system to go from z' to z'' is given by

$$\langle T \rangle = \mathcal{N}^{-1} \int_0^\infty T |K(z'', z', T)|^2 \, dT \,, \tag{15}$$

with

$$\mathcal{N} = \int_0^\infty |K(z'', z', T)|^2 \, dT \,, \tag{16}$$

which is the average total time. Similarly the time

$$\langle \Delta_\Omega \rangle = \mathcal{N}^{-1} \int_0^\infty \Delta_\Omega |K(z'', z', T)|^2 \, dT \tag{17}$$

is the average transition time within the region Ω.

In Fig. 3 we show the "isocronous" lines of the average times (17) for a part of the z'' plane shown in Fig. 2. In (17), the limits were set equal to $\tau_{\min} = 2.0$ and $\tau_{\max} = 5.5$ for which $|K(z'', z', T)|^2$ is sufficiently close to zero. Then, for each integral element in T, the propagator and $\Delta_\Omega(z'', z', T)$ were calculated. This figure gives the values of q'' and p'' for which the initial state with $q' = -7.0$, $p' = 4.0$, $c = 1.0$, and $b = 1.0$ has spent the same time within the barrier. As one can see, the average traversal time increases with p'', that is, the larger the final momentum, the longer the time the packet spends in the potential region. There is also a weaker dependence on the final q'', which shows that the farther the final point, the larger the value of Δ_Ω. This shows that there is still a residual interaction between the particle and the barrier due to both the width of the packet and the smoothed barrier in the studied region. A detailed analysis of the role of the width b and other barrier parameters, as well as comparisons between the traversal time proposed here and other definitions [1], will be published elsewhere.

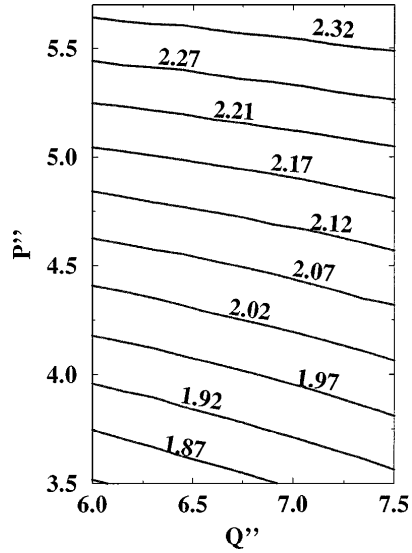

FIG. 3. Isocronous curves of $\langle \Delta_\Omega(z', z'') \rangle$ for the initial wave packet with $q' = -7.0$, $p' = 4.0$, $b = 1.0$, and $c = 1.0$ ($V_0 = 10.0$ and $a = 4.0$).

In summary, we have shown that the present semiclassical approximation for the coherent-state propagator $K(z'', z', T)$ leads to accurate calculations (with respect to the exact result). This approximation makes use of stationary trajectories which exist in a complexified phase space, but which propagate in real time. In this new space, the barrier is complex valued and smoothed. A new traversal time is then simply defined as the time spent in the potential region by the particle moving according to the complex trajectory from the initial position z' to z'' during the whole time T.

As a final remark we recall that Gaussian wave packets of minimum uncertainty are the closest quantum representations of classical particles. Therefore, the times measured along the related classical trajectories contributing to their evolution must be relevant in the semiclassical limit. Of course it is only in this limit that the concept of classical trajectories, and the very concept of time along them, makes any sense. We have shown here that the time spent by the trajectories in the barrier region can be computed even for average energies below the barrier height, constituting a sensible candidate for a tunneling time.

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