Tunneling of an energy eigenstate through a parabolic barrier viewed from Wigner phase space

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We analyze the tunneling of a particle through a repulsive potential resulting from an inverted harmonic oscillator in the quantum mechanical phase space described by the Wigner function. In particular, we solve the partial differential equations in phase space determining the Wigner function of an energy eigenstate of the inverted oscillator. The reflection or transmission coefficients \( R \) or \( T \) are then given by the total weight of all classical phase-space trajectories corresponding to energies below, or above the top of the barrier given by the Wigner function.

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1. Introduction

Tunneling [1] of a particle through a barrier is one of the striking phenomena of quantum mechanics [2]. In the special case of a repulsive quadratic potential, corresponding for example to an inverted harmonic oscillator [3] shown in Fig. 1(a), the transmission coefficient \( T \) takes the form [4]

\[ T = \frac{1}{1 + e^{-2\pi \varepsilon}}, \quad (1) \]

depicted in Fig. 1(b). Here \( \varepsilon \equiv E/(\hbar \Omega) \) is the scaled energy which is the ratio of the eigenvalue \( E \) and the natural energy parameter \( \hbar \Omega \), where \( \Omega \) is the steepness of the quadratic barrier and \( \hbar \) denotes the Planck constant divided by \( 2\pi \).

The expression Eq. (1) has played a crucial role in the context of nuclear fission [5]. It usually emerges [5] from a semiclassical analysis [6,7] of the Schrödinger equation of the inverted harmonic oscillator [3]. However, in the present Letter we rederive Eq. (1) from quantum phase space using the Wigner distribution function [8]. In particular, we show that Eq. (1) corresponds to the quantum mechanical weight of all classical trajectories [9] that have sufficient energy to go above the barrier.

This result is counterintuitive since in the standard formulation [2] of quantum mechanics à la Heisenberg and Schrödinger an energy eigenstate does not contain energies other than the eigenvalue. In contrast, the Wigner function [8] of such a state relies on the trajectories of all energies, however with positive or negative weights. Hence, the goal is to find these weights.

For this purpose we recall that two partial differential equations in phase space [10,11] determine the Wigner function of an energy eigenstate. They result from the commutator and the anti-commutator of the density operator with the Hamiltonian. The commutator yields the propagation equation of the Wigner function, that is, the quantum Liouville equation. In contrast, the anti-commutator leads to the phase-space analog of the Schrödinger eigenvalue equation.

For the case of an inverted harmonic oscillator the quantum Liouville equation reduces to the classical Liouville equation and is therefore, independent of \( \hbar \). In particular, it shows that the Wigner function of an energy eigenstate is constant along the classical trajectories. However, even for a quadratic barrier, the equation following from the anti-commutator contains \( \hbar \) explicitly. It is this equation which determines the quantum mechanical weight of each classical trajectory and provides us in this way with the tunneling and reflection coefficient.

This discussion also brings out most clearly the difference between a dynamical situation where a wave packet approaches a quadratic barrier and a stationary one corresponding to an energy eigenstate which is the topic of our Letter. Indeed, in the dynamical case, it is sufficient to propagate the Wigner function representing the initial wave packet along the classical trajectories as dictated by the reduction of the quantum Liouville equation to the classical. In this scenario \( \hbar \) enters only through the initial state.

However, for the analysis of the energy eigenstate the propagation equation does not suffice. We also need to invoke the phase-space analog of the Schrödinger eigenvalue equation.
analog of the Schrödinger eigenvalue equation the kernel of the 
at event horizons of black holes associated with logarithmic phase 
tation of the tunneling coefficient. Moreover, it also builds a bridge 
not only direct but also yields immediately the proposed interpre-
function from phase space. Therefore, we find the Wigner function 
to the quantum mechanical weight of all classical trajectories going above the bar-
approaching from the left. The quantum mechanical transmission curve (b) is due 
ing situations only half of phase space is accessible depicted in (d) for a particle 
trajectories coming from the left and from the right. Hence, under normal scatter-
being reflected from, stopping at the top of, or going above the potential hill, re-
the barrier — we depict the classical phase-space trajectories (c) which are either 
from the left (d). For three different energies — below, at the top of, and above 
phase-space trajectories (c) subjected to the boundary conditions of a particle com-
parabolic barrier (a) in its dependence on 
expressed by the Hamiltonian
\[ H \equiv \frac{p^2}{2M} - \frac{1}{2} M \Omega^2 x^2. \] (2)
Here \( x \) and \( p \) denote the position and the coordinate of the particle.

For this purpose we consider the Wigner function [8]
\[ W_E(x, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \ e^{-ipy/\hbar} \psi_E^* \left( x - \frac{y}{2} \right) \psi_E \left( x + \frac{y}{2} \right) \] (3)
of an energy eigenstate \( |E\rangle \) of \( \hat{H} \) with wave function \( \psi_E(x) \). However, instead of solving first the time independent Schrödinger equation \( \hat{H} \psi_E = E \psi_E \) for \( \psi_E \) and then performing the integration in Eq. (3) pursued in Ref. [12], we analyze the partial differential equations [10,11]

\[
\frac{p}{M} \frac{\partial}{\partial x} + M \Omega^2 x \frac{\partial}{\partial p} W_E(x, p) = 0
\] (4)
and
\[
\left( \frac{p^2}{2M} - \frac{1}{2} M \Omega^2 x^2 \right) - \frac{\hbar^2}{8} \left( \frac{1}{M} \frac{\partial^2}{\partial x^2} - M \Omega^2 \frac{\partial^2}{\partial p^2} \right) W_E(x, p) = E W_E(x, p)
\] (5)
for the Wigner function in phase space. We emphasize that Eqs. (4) and (5) are exact for the inverted harmonic oscillator.

3. Wigner function

The classical Liouville equation (4) implies that \( W_E \) is constant along the classical phase-space trajectories of a fixed energy \( H \) given by Eq. (2) and shown in Fig. 1(c), that is
\[ W_E(x, p) = \mathcal{W}_E/(\hbar \Omega) \left( \frac{H(x, p)}{\hbar \Omega} \right). \] (6)

Next we take into account the boundary conditions associated with a scattering process. Two distinct possibilities offer themselves: (i) the particle approaches the barrier from the left, or (ii) it impinges from the right.

The two cases manifest themselves in different classical phase-space trajectories. Whereas the situation (i) is described by the trajectories in the domain above the separatrix
\[ p = M \Omega x, \] (7)
depicted in Fig. 1(d), the case (ii) covers the area below it.

Hence, for a particle coming from the left, the Wigner function \( W_E^{(l)} \) of an energy eigenstate reads
\[ W_E^{(l)}(x, p) = \mathcal{W}_E/(\hbar \Omega) \left( \frac{H(x, p)}{\hbar \Omega} \right) \Theta(p - M \Omega x), \] (8a)
where \( \Theta \) denotes the Heaviside step function. Hence, only the classical trajectories above the separatrix contribute to the Wigner function as shown in Fig. 1(d).

Likewise, for a particle approaching from the right we find
\[ W_E^{(r)}(x, p) = \mathcal{W}_E/(\hbar \Omega) \left( \frac{H(x, p)}{\hbar \Omega} \right) \Theta(M \Omega x - p). \] (8b)

With the help of the familiar identity
\[ \delta(x) = 0 \] (9)
for the Dirac delta function it is easy to verify that both expressions satisfy the Liouville equation (4) as long as the function \( \mathcal{W}_E \) is differentiable. The form of \( \mathcal{W}_E = \mathcal{W}_E^{(l)}(t) \) corresponding to the scaled eigenvalue \( \varepsilon \equiv E/(\hbar \Omega) \) in its dependence on the dimensional energy
\[ \eta \equiv \frac{H(x, p)}{\hbar \Omega} = \frac{1}{\hbar \Omega} \left[ \frac{p^2}{2M} - \frac{1}{2} M \Omega^2 x^2 \right] \] (10)
of a classical trajectory is then determined by the Schrödinger equation (5) in phase space. Indeed, when we substitute the ansatz Eq. (8b) into Eq. (5) we arrive at the ordinary differential equation
\[ \eta \frac{d^2 \mathcal{W}_E}{d\eta^2} + \frac{d\mathcal{W}_E}{d\eta} - 4(\varepsilon - \eta) \mathcal{W}_E = 0. \] (11)
Again we have made use of Eq. (9). It is remarkable that Eq. (11) is independent of the Heaviside step function.
In order to solve Eq. (11) we make a Fourier ansatz

$$\mathcal{W}_e(\eta) \equiv \int_{\tau_1}^{\tau_2} d\tau \, W_e(\tau) e^{i\eta \tau}$$

(12)

where the limits $\tau_1$ and $\tau_2$ of the integration will be determined in a way as to simplify the differential equation for $W_e = W_e(\tau)$ resulting from (11). Indeed, with the integral relation

$$\eta \mathcal{W}_e(\eta) = \int_{\tau_1}^{\tau_2} d\tau \, W_e(\tau) \left( \frac{1}{i} \partial_{\tau} + \eta \right) e^{i\eta \tau}$$

(13)

and integration by parts we establish the identity

$$\eta \mathcal{W}_e(\eta) = \frac{1}{i} \left[ W_e(\tau_2) e^{i\eta \tau_2} - W_e(\tau_1) e^{i\eta \tau_1} \right]$$

$$- \frac{1}{i} \int_{\tau_1}^{\tau_2} d\tau \, \frac{d}{d\tau} \left[ W_e(\tau) \right] e^{i\eta \tau}$$

(14)

Similarly, we obtain

$$\eta \frac{d^2 \mathcal{W}_e}{d\eta^2} = -\frac{1}{i} \left[ W_e(\tau_2) 2\tau_2 e^{i\eta \tau_2} - W_e(\tau_1) 2\tau_1 e^{i\eta \tau_1} \right]$$

$$+ \frac{1}{i} \int_{\tau_1}^{\tau_2} d\tau \, \frac{d}{d\tau} \left[ \tau^2 W_e(\tau) \right] e^{i\eta \tau}$$

(15)

and

$$\frac{d\mathcal{W}_e}{d\eta} \bigg|_{\tau_1}^{\tau_2} = \int_{\tau_1}^{\tau_2} d\tau \, i \tau W_e(\tau) e^{i\eta \tau},$$

(16)

which when substituted into (11) yields the ordinary differential equation

$$i(4 - \tau^2) \frac{dW_e}{d\tau} - (i\tau + 4\epsilon) W_e = 0$$

(17)

of first order for $W_e = W_e(\tau)$. Here we have made the choice $\tau_1 \equiv -2$ and $\tau_2 \equiv 2$ which eliminates the boundary terms in Eqs. (14) and (15).

By direct differentiation we can verify that

$$w_e(\tau) \equiv A (4 - \tau^2)^{-1/2} \exp\left[ -i\epsilon \ln\left( \frac{2 + \tau}{2 - \tau} \right) \right]$$

(18)

is a solution of Eq. (17) and the constant

$$A \equiv \frac{1}{\pi}$$

(19)

of integration follows from the normalization condition

$$1 = \int_{-\infty}^{+\infty} d\eta \, \mathcal{W}_e(\eta)$$

(20)

which is a consequence of the Fourier ansatz Eq. (12).

As a result, the crucial part $\mathcal{W}_e$ of the Wigner function of an energy eigenstate of the inverted harmonic oscillator reads

$$\mathcal{W}_e(\eta) = \frac{1}{\pi} \int_{-2}^{2} d\tau \, \frac{\exp(-i\epsilon \ln(2 + \tau)(2 - \tau))}{\sqrt{4 - \tau^2}} e^{i\eta \tau}.$$  

(21)

Fig. 2. The Wigner function $W^{(0)}_e$ of an energy eigenstate of the inverted harmonic oscillator for the dimensionless energy $\epsilon = -0.4$ that is below the top of the barrier and corresponding to a particle coming from the left. Due to this boundary condition the Wigner function vanishes in the phase-space domain above the separatrix (right upper part). It is constant along the classical trajectories with a dominant maximum at the trajectory corresponding to the energy eigenvalue (front). However, the Wigner function also reaches into the domain of trajectories traversing the barrier (left). The total weight underneath the Wigner function in this realm represents the tunneling coefficient.

Since our ultimate goal is to calculate the transmission and reflection coefficients we do not discuss this expression in more detail but emphasize that $\mathcal{W}_e$ is real and satisfies the symmetry relation

$$\mathcal{W}_{-e}(-\eta) = \mathcal{W}_e(\eta).$$

(22)

In Fig. 2 we depict the Wigner function of the energy eigenstate of an inverted harmonic oscillator below the top of the barrier subjected to the initial condition of the particle approaching from the left represented by Fig. 1(d). In order to bring out the characteristic features we have rotated the phase space by 90°. The wave fronts in the foreground correspond to the phase-space trajectories of particles coming in and being reflected from the barrier. The waves on the upper left of the figure with much reduced amplitude represent particles going above the barrier. In the flat part above the separatrix extending to the right upper corner the Wigner function vanishes as to obey the boundary condition corresponding to the gray shaded area in Fig. 1(d).

4. Reflection and transmission coefficients

We now turn to the evaluation of the transmission probability $T$ which is given by the integral

$$T \equiv \int_{0}^{\infty} d\eta \, \mathcal{W}_e(\eta)$$

(23)

of the Wigner function over positive values of $\eta$ only.

With the help of the identity

$$\int_{0}^{\infty} d\eta \, e^{i\eta \tau} = \pi \delta(\tau) + i\mathcal{P}\left( \frac{1}{\tau} \right)$$

(24)

we find from Eq. (21) the expression

$$T = \frac{1}{2} + \frac{i}{4\pi} \mathcal{P} \left[ \int_{-\infty}^{+\infty} d\xi \, \frac{\exp(-i\epsilon \xi)}{\sinh(\xi/2)} \right].$$

(25)

where we have introduced the new integration variable $\xi \equiv \ln((2 + \tau)/(2 - \tau))$ and $\mathcal{P}$ denotes the Cauchy principal part.

1 With the transformation $\tau = 4t - 2$ this integral reduces to the integral representation of the Kummer function.
Due to the antisymmetry of $\sinh(\xi/2)$ only the imaginary part survives, that is

$$T = \frac{1}{2} \left[ 1 + \frac{1}{\pi} \int_0^\infty d\xi \frac{\sin(\xi)}{\sinh(\xi/2)} \right]$$

(26)

and with the integral relation [13]

$$\int_0^\infty d\xi \frac{\sin(\xi)}{\sinh(\beta\xi)} = \pi \tanh\left(\frac{\xi\pi}{2\beta}\right)$$

(27)

we finally arrive at

$$T = \frac{1}{2} \left[ 1 + \tanh(\xi\pi) \right]$$

(28)

in complete agreement with Eq. (1).

We conclude by noting that the reflection coefficient $R$ follows from the identity

$$R + T = 1,$$

(29)

together with the normalization condition Eq. (20) and the definition Eq. (23) of $T$,

$$R = \int_0^\infty d\eta \mathcal{W}_E(\eta).$$

(30)

Therefore, it is the total quantum mechanical weight of the classical trajectories that are reflected, that is all energies below the maximum of the barrier.

5. Summary and outlook

In summary, we have rederived the familiar reflection and the tunneling coefficients $R$ and $T$ for an inverted harmonic oscillator using the corresponding Wigner function. This approach shows that $R$ and $T$ represent the quantum mechanical weights given by the Wigner function of all classical trajectories that are reflected or transverse the barrier as indicated in Fig. 3. The weight of a given trajectory follows from an ordinary differential equation of second order which we have solved using a Fourier representation of the Wigner function.

Here we have not analyzed in detail the structure of the resulting differential equation of first order given by Eq. (17) in the complex plane. It suffices to say, that the origin of Eq. (1) is deeply rooted in the two poles at $\tau = -2$ and $\tau = 2$ giving rise to a logarithmic phase singularity [14] contained according to Eq. (18) in the kernel $\mathcal{W}_R$ of the Fourier representation of $\mathcal{W}_E$.

Such singularities also appear [3,12] in the quadrature representation of the energy wave function and manifest themselves in the Unruh effect [15], the Hawking radiation [16] or optical analogues [17] of event horizons of black holes. To identify in the complex plane the crucial contributions to the integral Eq. (12), or to elaborate on the importance of the logarithmic singularity, and to compare and contrast the similarities and differences between tunneling and particle creation goes beyond the scope of this letter and will be the topic of a future publication.

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