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Probabilities for Quantum Tunneling through a Barrier with Linear Passive Dissipation

A. Widom

Physics Department, Northeastern University, Boston, Massachusetts 02115

and

T. D. Clark

Physics Laboratory, University of Sussex, Brighton BN1 9QH, Sussex, England (Received 9 June 1981)

The transmission coefficient for passage through a barrier with a parabolic maximum is computed rigorously when linear passive dissipation is present. The exact result for energies above and below the barrier height can be expressed in terms of the Coleman renormalized one-bounce time. The quasiclassical (WKB) approximation is recovered for energies significantly below the barrier height where "friction" enhances the tunneling probability.

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There has been considerable recent interest in the quantum mechanical tunneling of a macroscopic coordinate through an energy barrier. In the neighborhood of a barrier maximum, the influence of linear passive dissipation has been discussed by Caldeira and Leggett.¹ This was in the context of the Kac-Feynman-Schwinger model of oscillator-bath couplings.² The quantum kinetics of such models has been reviewed by Benguria and Kac.³

The principal conclusion of Caldeira and Leggett is that dissipative oscillator-bath couplings decrease the quantum mechanical tunneling probability. Their calculation relies on the WKB approximation and the Coleman one-bounce dynamics.⁴

The purpose of this work is to exhibit the rigorously exact expression for the transmission probability through a barrier with linear passive dissipation and a parabolic maximum. We find that the rigorous solution has the following properties: (i) The Coleman one-bounce time determines the quantum mechanical transmission probability in all regimes, not just in the WKB limit. (ii) The dissipative oscillator-bath couplings strictly increase the probability of quantum mechanical tunneling.

We attribute the qualitative difference between the Caldeira-Leggett conclusions and the rigorous results (which follow) to an incorrect treatment of renormalizations which lead to divergences in their theory. For dissipative processes with a finite oscillator-strength sum rule, no divergence appears in the exact calculation.

The transmission probability through a barrier with a parabolic maximum for a single degree of freedom, i.e.,

$$h = -(\hbar^2/2m)(d/dx)^2 - \frac{1}{2}m\Omega_0^2 x^2, \qquad (1)$$

is a well-known quantum mechanical problem⁵ whose history is closely intertwined with the WKB quasiclassical computational scheme.⁶ In terms of the oscillation period of the coordinate x (in a situation where the parabola is formally

inverted),

$$\tau_{0} = (2\pi/\Omega_{0}), \qquad (2)$$

the rigorous expression for the quantum mechanical transmission probability is given by

$$P_{0}(E) = \left[1 + \exp(-E\tau_{0}/\hbar) \right]^{-1}$$
(3)

for all energies above (E > 0) or below (E < 0) the energy at the barrier maximum. The only mathematically subtle point in deriving Eq. (3) from the Hamiltonian in Eq. (1) is the boundary condition on the wave function far from the barrier classical turning point. This has been discussed in the literature.^{7,8}

Now let us discuss the many-body Hamiltonian

$$H = h + \frac{1}{2} \sum_{k} (P_{k}^{2} + \omega_{k}^{2} Q_{k}^{2}) + \sum_{k} \lambda_{k} Q_{k} x, \qquad (4)$$

where linear dissipative coupling into an oscillator bath induces a linear passive "friction coefficient" $\Gamma(\zeta)$, analytic in the upper half of the complex frequency plane. The potential energy surface in configuration space, which in the absence of oscillator-bath coupling was an inverted parabola, now appears as a "saddle" with a single unstable direction. The imaginary frequency,

$$\zeta - \pm i\Omega, \tag{5}$$

of the unstable saddle direction (in the thermodynamic limit of "dense oscillator-bath spectra") can be found from the dissipative part of the friction coefficient via the analyticity dispersion relation for $\Gamma(\zeta)$; the equation for Ω is

$$\Omega^{2} = \Omega_{0}^{2} + (2/\pi) \int_{0}^{\infty} d\omega \, \omega^{2} \operatorname{Re} \Gamma(\omega + i0^{+}) / (\omega^{2} + \Omega^{2}) \,.$$
(6)

A sufficient condition for the validity of Eq. (6) in determining a unique "one-bounce" Coleman (saddle) time,⁴

$$\tau = (2\pi/\Omega), \tag{7}$$

is that the oscillator-strength sum rule,

$$\nu^{2} = (2/\pi) \int_{0}^{\infty} d\omega \operatorname{Re} \Gamma(\omega + i0^{+}), \qquad (8)$$

yield a "well defined" (i.e., finite) value of ν . This condition is evidently consistent with models for which the zero-frequency friction coefficient exists,

$$\gamma = \lim_{\omega \to 0} \operatorname{Re} \Gamma(\omega + i0^{+}), \qquad (9)$$

as long as no high-frequency divergence enters into the integral in Eq. (8).

For systems with any positive dissipative spectral weight, one notes that Eqs. (6) and (8) imply the inequalities

$$\Omega^2 > \Omega_0^2, \tag{10a}$$

$$\Omega^2 < (\Omega_0^2 + \nu^2) \,. \tag{10b}$$

In terms of the one-bounce times τ (with dissipation) and τ_0 (without dissipation), Eqs. (10) read

$$\tau < \tau_0$$
, (11a)

$$\tau > \tau_0 \left[1 + \nu^2 \tau_0^2 \right]^{-1/2}.$$
 (11b)

By a linear transformation which mixes the tunneling coordinate x with the oscillator coordinates $\{Q_k\}$, the potential "saddle" in configuration space can be reduced to principal directions, only one of which corresponds to the quantum tunneling process while the rest describe normal, independent, stable oscillator modes. The tunneling problem in the unstable saddle direction is formally one dimensional with a probability of transmission

$$P(E) = \left[1 + \exp(-E\tau/\hbar) \right]^{-1}.$$
 (12)

Equations (1), (4), (6), (7), and (12) reduce to quadratures the problem of barrier transmission (for all E) in the neighborhood of a parabolic maximum with a frequency-dependent damping $\operatorname{Re}\Gamma(\omega+i0^+)$. The WKB regime is contained in Eq. (12) as the asymptotic form

$$P(E) \to \exp(-|E|\tau/\hbar), \quad E \to -\infty.$$
(13)

However, it is evident that the complete solution in Eq. (12) determines P(E), via the formal onebounce time τ , for all E.

From Eqs. (3), (11a), and (13) one reaches the following conclusions. (i) In the quantum tunneling regime, dissipation increases the barrier transmission probability:

$$P(E) > P_0(E), \quad E < 0.$$
 (14)

(ii) For energies above the barrier height, dissipation increases the reflection probability R = 1 - P, i.e.,

$$P(E) < P_{o}(E), \quad E > 0.$$
⁽¹⁵⁾

(iii) For an energy E = 0, equal to the barrier height, the transmission and reflection probabilities are both $\frac{1}{2}$.

In the work of Caldeira and Leggett¹ the conclusion reached was that dissipation lowered the transmission probability in the quantum tunneling regime. We attribute the difference between the results here reported and those of Caldeira and Leggett to a divergent renormalization which VOLUME 48, NUMBER 2

they state is "unobservable." This appears (in our view) from the divergence in the oscillatorstrength sum rule implicit in their calculational method. For a finite total oscillator strength in, for example, electrical conductivity applications, no divergent terms are expected to appear physically in the calculation. For example, in a finite-oscillator-strength Drude model, the friction coefficient reads

$$\Gamma(\zeta) = \left[\nu^2 \tau^* / (1 + i\zeta\tau^*) \right].$$
(16)

For such a model, a sufficient condition for dissipation to be unimportant for barrier transmission is that

$$\gamma \tau_0^2 \ll \tau^* \text{ (underdamped)},$$
 (17)

where $\gamma = \nu^2 \tau^*$ is the zero-frequency friction coefficient [Eq. (9)] and τ_0 is the "friction-free" one-bounce time. Quantum tunneling enhancement for E < 0 is expected when

 $\gamma \tau_0^2 \gg \tau^*$ (overdamped).

Note added.—Had we chosen a potential barrier with an energy lower bound, then a rigorous

solution would be difficult to obtain. Nevertheless the following theorem on the WKB barrier factor can be proven: Since the barrier factor is the *minimum* action through an "inverted potential region," any additional fluctuating coordinates *lower* the barrier factor, i.e., *increase* the transmission coefficient. This general theorem is in qualitative physical agreement with the above rigorous model.

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