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Dissipative quantum tunneling at finite temperatures

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Finite temperatures are incorporated into the calculation of the tunneling rate in the presence of linear dissipation. A theory of finite-temperature tunneling is introduced which is based on the density matrix which provides an approximate description of the metastable state. Semiclassical functional integral methods are used to calculate the density matrix and the Wentzel-Kramers-Brillouin approximation is used to derive the tunnel current from the density matrix. Dissipation appropriate to superconducting quantum-interference devices is introduced into the calculation by the use of the existing model of a heat bath consisting of a prescribed distribution of harmonic oscillators linearly coupled to the tunneling variable. The finite-temperature tunnel escape rate obtained is of the form $\Gamma = A \exp(-S/\hbar)$. S is determined from the solution of a nonlinear integro-differential equation. An existing numerical technique was modified to achieve this. The quantity A is approximately evaluated.

I. INTRODUCTION

The problem of escape of a physical system trapped in a metastable potential well is one with many exemplifications in physics and chemistry. Well-known examples include the decay of a heavy nucleus by emission of an α particle, the field emission of an electron from an atom or from a solid surface, many chemical reactions, and the motion of paraelectric defects in an insulating solid. In these cases the systems in question are microscopic. However, thanks to the rapid development of cryogenic technology, it has also become possible in recent years to study cases where the "trapped" variable is macroscopic: for example, the magnetic flux through an rf SQUID ring, or the charge-density waves in certain one-dimensional solids. The considerations presented in this paper were developed with reference primarily to such a macroscopic context.

At high temperatures the process by which the system escapes from the metastable well is of course the classical Kramers[1] process, in which it picks up enough energy, by a thermodynamic fluctuation, from its environment to surmount the barrier in a purely classical manner. In his original calculation, Kramers considered a system with coordinate $q(t)$ which was subject to random noise exerted by its environment in such a way that its equation of motion contained a frictional force $-\eta\dot{q}$. He showed that the rate of escape was given by a formula of the general form

$$P = \omega(\eta, T)\exp(-V_0/k_B T) , \tag{1.1}$$

where V_0 is the height of the potential barrier (measured relative to the bottom of the metastable well) and $\omega(\eta, T)$ is a quantity with dimensions of frequency, which in his model tends to zero in the limit both of very small and of very large friction η. This is easy to understand physically: for large friction the system diffuses over the barrier only very slowly, while for weak friction it has difficulty in picking up enough energy from the environment to surmount the barrier. In the present context it is important to emphasize two points: (1) the escape rate [Eq. (1.1)] depends only on the height of the barrier, not on its width or shape, and (2) in the absence of any friction at all the escape rate is strictly zero [since the prefactor $\omega(\eta, T)$ vanishes]. While these general features of Kramers's solution have been confirmed by subsequent work on the subject, there is still a certain amount of debate on the prefactor in the intermediate domain: see, e.g., Ref. 2 and the literature cited therein.

At low enough temperatures the Kramers's formula gives a negligible escape rate, and the principal mechanism by which the system can leave the metastable well is by quantum tunneling through the barrier. If our system is *totally isolated* from any environment, then the standard Wentzel-Kramers-Brillouin (WKB) formulas should apply; the tunneling rate at zero temperature is given by the following expression [In Eq. (1.2) the WKB integral is taken between the classical turning points for a particle of zero energy. It is of course also possible to write it in terms of the integral between turning points for one of energy $\hbar\omega_0/2$: this merely introduces an extra $\hbar$-independent factor into ω_a.]:

$$P = \omega_a \exp\left[-2\int_0^{q_0} [2MV(q)]^{1/2} dq/\hbar\right] , \tag{1.2}$$

where M is the mass of the system and q_0 is the "exit point" from the barrier, i.e., the first nonzero value of q at which $V(q)=0$. [We take the metastable minimum to lie at $q=0$, $V(0)=0$.] The prefactor ω_a in Eq. (1.2) is of the order of the small oscillation frequency $\omega_0=[V''(0)/M]$ [times a factor of order $(V_0/\hbar\omega_0)^{1/2}$].

Note that in contrast to the Kramers formula Eq. (1.1) the WKB expression [Eq. (1.2)] (1) depends on the width and shape of the barrier as well as its height and (2) is perfectly finite in the limit of zero friction. Since it is obvious after a little dimensional analysis that the WKB exponent in Eq. (1.2) can be written for any nonpathological potential in the form $\alpha V_0/\hbar\omega_0$, where α is typically of order 2π, we see that the Kramers rate calculated from Eq. (1.1) becomes comparable to the zero-temperature tunneling rate when the condition $k_B T \approx \hbar\omega_0/2\pi$ is satisfied. Consequently if we are interested primarily in quantum effects, we should restrict ourselves to temperatures lower than this (cf. however, Refs. 3–5).

We may now ask how the expression of Eq. (1.2) is to be generalized to low but finite temperatures. As regards the dominant exponential factor, the answer is straightforward, at least provided we assume that the barrier height V_0 is sufficiently large compared with $\hbar\omega_0$. If this is so, the well will contain many excited states which in the absence of tunneling would be energy eigenstates, and in the limit $V_0/\hbar\omega_0 \to \infty$ it is natural to approximate these by a continuum. We then pose the question as follows: if at time zero the population of these states was described by a Boltzmann distribution at temperature $T \equiv (k_B\beta)^{-1}$, what is the initial rate at which the probability of finding the particle in the well decays? To answer this question we note that the probability of decay from an excited state of energy E is given by the formula

$$\Gamma(E) = \omega_a(E) \exp\left[-2\int_{q_1}^{q_2} [2MV(q)]^{1/2} dq/\hbar\right], \tag{1.3}$$

where the prefactor $\omega_a(E)$ is a slowly varying function of E. As is well known[6] the WKB exponent can also be written in the form $A(E)/\hbar$ where A is the classical action ($\int pdq$) of a particle of energy $-E$ performing a complete periodic motion in the *inverted* potential $V(q) \equiv -\tilde{V}(q)$. Since the probability of the system being in a state of energy E is $Z_0^{-1}\exp(-\beta E)$ where Z_0 is the partition function, the total decay probability is

$$\Gamma = Z_0^{-1} \int_0^\infty dE\, \rho(E)\omega_a(E) \exp[-A(E)/\hbar]\exp(-\beta E), \tag{1.4}$$

where $\rho(E)$ is the density of levels with respect to energy. If we neglect the slow variation of the factor $\rho(E)\omega_a(E)$ the expression (1.4) is dominated by the minimum of the exponent $\beta E + A(E)/\hbar$, which occurs at an energy given by $\beta = -\hbar^{-1}\partial A/\partial E$. Recalling that A is actually the classical action of a trajectory with energy $-E$ in the inverted potential, we have $-\partial A/\partial E = \tau$ where τ is the period of the classical motion in question. Thus, the dominant tunneling takes place at or near the energy such that $\tau(E) = \beta\hbar$. Since, for any reasonably smooth form of the potential, the quantity $\tau(E)$ decreases smoothly from the value infinity for $E=0$ to the value $2\pi/\omega_0'$ for $E \to V_0$ where ω_0' is the quantity $(-V''/M)^{1/2}$ evaluated at the *top* of the barrier, it follows that the equation $\tau(E) = \beta h$ has a solution only for $\beta\hbar\omega_0'/2\pi > 1$, i.e., for $k_B T \ll \hbar\omega_0'/2\pi = k_B T_0$. At temperatures higher than this the main contribution to the decay probability comes not from tunneling but from classical fluctuation processes taking the system *over* the barrier, in accordance with the order-of-magnitude estimate derived above (since $\omega_0 \approx \omega_0'$ for not too pathological forms of potential). We shall not explore this region here (although cf. the remarks below).

The upshot of the above discussion is that the argument of the exponential factor in the tunneling rate is the quantity $\beta E + A(E)/\hbar$ evaluated along that classical cyclic path in the inverted potential which is traversed in a time $\tau = \beta\hbar$, where E is the energy appropriate to this path. Since in classical mechanics the quantity $E\tau + A(E)$ is just the time integral of the Lagrangian along the path, we can write the result in the form

$$\Gamma = f(T)\exp(-S/\hbar), \tag{1.5}$$

$$S = \int L(q,\dot{q})dt, \tag{1.6}$$

where the quantity S is evaluated along the "classical" path determined as above and $f(T)$ is a quantity which is not exponentially sensitive to $\hbar$. In the literature on tunneling it is common to see S referred to as the classical action; we shall adopt this usage since no confusion is likely to occur.

The question of the prefactor is more subtle. In Ref. 7, Affleck took the quantity $\rho(E)\omega_a(E)$ to have the constant value $(2\pi\hbar)^{-1}$ and thereby derived for the prefactor the expression $Z_0^{-1} \mid 2\pi\hbar\partial\tau/\partial E \mid^{-1}$. He showed that Eq. (1.5) with this value of $f(T)$ is also obtained if we assume the relation

$$\Gamma = \frac{2}{\hbar}\mathrm{Im}F(T), \tag{1.7}$$

where F is the free energy at temperature T.

A point which will be of considerable importance in the generalization to dissipative systems (see below) is that, *for the model studied,* that is, for a system which is assumed totally decoupled from the rest of the universe but nevertheless described initially by a Boltzmann distribution as regards the excited states in the metastable well, the above results are correct only for the *initial* decay rate. The reason is trivial: for finite (real) time t the prediction of this model for the probability $P(t)$ that the system is still to be found in the metastable well is

$$P(t) = Z_0^{-1}\int \rho(E)\exp(-\beta E)\exp[-\Gamma(E)t]dE, \tag{1.8}$$

so that $\Gamma(t) = -(d/dt)\ln P(t)$ is in general not even constant in time. Now, of course, the obvious reply is that it is not realistic to decouple the system so completely from its environment that the Boltzmann distribution is not obtained; rather, the physically realistic assumption is that weak but finite interactions maintain the relative populations of the states in the well at its Boltzmann form for all times, in which case the above argument [and in particular Eq. (1.5)] should predict the decay probability correctly for all t. While this argument has considerable plausibility, and it would be very surprising if the exponential factor in Eq. (1.5) were wrong, it is by no means clear that the *prefactor* is correctly given. Indeed as explicitly noted by Affleck,[7] use of the analogous formula well above the crossover temperature T_0 correctly reproduces the Kramers exponent $-\beta V_0$ but gives the prefactor $\omega_0/2\pi$ corresponding to the "transition-state" theory; the latter is gen-

erally believed to give quite incorrect results for the *steady-state* rate in the weak damping limit. (In particular, quite general arguments would indicate that in the limit where the damping tends to zero the prefactor should also tend to zero, as it indeed does in the Kramers theory.) Thus *even for the undamped case* the use of formula (1.7) for the steady-state rate is not completely free of problems.

Two further points need to be briefly noted about the arguments leading to Eq. (1.5). First, we had to assume that the energy levels in the well could be approximated by a continuum. As a matter of fact, this is almost always a rather poor approximation in cases of physical interest, since even for, say, the fission of ^{238}U the quantity $V_0/\hbar\omega_0$ is only of order 10 while for systems such as SQUID rings it may easily be only 2 or 3. In such cases a more detailed calculation is needed and the results[8,9] show differences from the predictions of Eq. (1.5) which are not negligible when comparison with experiment is made; in particular, the smooth temperature dependence predicted by Eq. (1.5) is replaced by a rather sharp kink (see Ref. 10, Fig. 4). This point relates primarily to the exponent. A related, although not identical point concerns the use of the approximation $(2\pi\hbar)^{-1}$ for the quantity $\rho(E)\omega_a(E)$ which helps to determine the prefactor. This should certainly be valid for states in the correspondence limit, but is not obviously so for the ground state and first few excited states. Thus, the applicability of formula (1.5) to situations of real-life experimental interest is not completely clear.

After this litany of scepticism we turn to the real subject of this work, namely the generalization of the above results to systems subject to appreciable dissipation. We refer, e.g. to Ref. 10 for a discussion of why this is an important question in particular in the context of tests of quantum mechanics at the macroscopic level, and hence assume its interest. We shall further *assume* in this paper that in the case under consideration the mechanism of dissipation can be adequately described by the "standard" model of linearly coupled harmonic oscillators introduced in Eq. (4.1) below. It should be emphasized that while strong arguments can be given[11] that this is an adequate general description in the case of zero-temperature tunneling, some of these arguments do not generalize trivially to the finite-temperature case, so that the validity of Eq. (4.1) as a general model of finite T requires separate discussion. Nevertheless, to the best of our knowledge all other work in this area which attempts to treat the *general* problem of tunneling in a linearly dissipative system at finite temperature (as distinct from work[12,13] on specific systems such as ideal tunnel-oxide junctions) has in effect started from the Lagrangian of Eq. (4.1). Thus, our problem, in common with that of other workers, is to determine the rate of tunneling of a "system" described by a coordinate q out of the metastable minimum of its potential $V(q)$, when it is coupled to an "environment" in the way described by Eq. (4.1). In this paper we shall furthermore (a) confine ourselves to the temperature region where classical above-barrier processes do not play a role (thus we shall not be concerned with the interesting question[3–5] of how quantum-mechanical effects modify the classical Kramers theory in the presence of appreciable dissipation for $T > T_0$, nor with the precise form of the classical behavior), and (b) specialize to the case of linear "Ohmic" dissipation [Eq. (4.4)] which is probably the case of most relevance in the context of macroscopic systems.

The generalization of these results to the case where constraint (b) is relaxed is straightforward (cf. Ref. 14); when (a) is relaxed it is rather less so, and we shall not attempt to discuss it here. In evaluating our formulas numerically we shall specialize even further, to the case of a quadratic plus cubic potential, which as explained in Ref. 11 is likely to be of most importance for macroscopic systems.

For the special case of zero temperature this problem was treated by Caldeira and one of us[15,11] and by others.[16–18] By contrast, when we started the work reported in this paper there were no results in the literature on the finite-temperature generalization. In the last year and a half or so, however, at least three different sets of workers[19–23] have reported extensive calculations on this problem; in particular, rather detailed quantitative expressions for both the exponent and the prefactor in the expression for the tunneling probability have been given by Larkin and Ovchinnikov[21] and by Grabert and Weiss[23] (however neither of these analyses was available to us when the work reported here was first presented[24]). The reader might well wonder what we have to add to these results.

In fact, the main reason why we think it worth publishing the results of our own calculations on this problem is that they are obtained by a method which is quite different from that used by other authors, and which we believe may avoid some of the conceptual difficulties in other approaches. In particular, the results of both Larkin and Ovchinnikov[20,21] and Grabert and Weiss[22,23] (the results of Zwerger[19] are difficult to compare with these, as he confines himself to weak damping and calculates the rate of tunneling out of the individual levels rather than the overall decay rate of the metastable state) are based on the use, for a dissipative system, of the formula (1.7), that is

$$\Gamma = \frac{2}{\hbar}\mathrm{Im}F \ . \tag{1.9}$$

While this identification is certainly a plausible one, no rigorous proof exists (to our knowledge) that it is correct for a dissipative system in the quantum regime.[25] In Ref. 20 it is justified implicitly by an analytic continuation procedure whose validity seems to us difficult to assess, while in Ref. 21 it is simply stated, with reference made to three papers, none of which deals with a dissipative system in the quantum tunneling regime. The authors of Ref. 23, by contrast, give explicit arguments in favor of the identification Eq. (19), namely that it reproduces results obtained by other means, and generally believed to be correct as follows: (a) for the nondissipative case (Ref. 7), (b) further in the limit of zero temperature (Ref. 11), (c) for temperatures above the crossover temperature T_0 to Kramers-like behavior (Ref. 4), and (d) for T slightly less than T_0. While these arguments are certainly attractive, it should perhaps be pointed out that in at least some of these cases the results with which comparison is made are

themselves not completely beyond doubt; see, in particular, the comments made above about case (a). [Further discussions of the significance and regions of validity of the relation (1.9) in the *classical* case has been given recently by Zwerger.[26] A further recent development of interest is by Dorsey and Fisher[27] and independently by Grabert and Weiss[28] which demonstrates that for the case of overdamped transitions in a slightly biased two-state problem, a calculation based on analytic continuation of the expression for the free energy gives results identical to those obtained from a real-time calculation. However, it is not clear how far this result is relevant to the present problem.] For this reason, in our own work we have consciously and deliberately avoided the use of formula (1.9) and attempted to obtain an expression for the tunneling rate Γ by a completely different method which requires no analytic continuation of any physical quantity at any stage of the calculation. While it does require the use of one unproved assumption [Eq. (4.28)], we believe that this assumption is no less plausible than that involved in the identification of Eq. (1.9). Thus if the results obtained in this way should agree with those obtained from Eq. (1.9), we could regard this as further support for the correctness of the latter (see, however, the Conclusion); if they should disagree, further analysis of both methods is clearly needed. Unfortunately, the question of the extent of agreement or disagreement is at the time of writing still rather unclear (see Conclusion). It should be emphasized that the disagreement, if any, is confined to the prefactor in the tunneling expression: our results for the exponent are identical to those of other authors. A second reason why we believe that this work may be of interest is that, in contrast to other authors who have evaluated the exponent analytically in certain limits, we have carried out a fairly extensive numerical evaluation for a wide range of values of dissipation and temperature, which we believe may complement the analytic work. These results were first presented in a thesis to the University of Sussex.[24]

The work presented in this paper is arranged as follows. In Sec. II we begin our approach to tunneling by deriving the approximate density matrix which describes the metastable state in the absence of dissipation. In Sec. III we show how to calculate the finite-temperature tunnel escape rate (in the absence of dissipation) from this density matrix. In Sec. IV the nondissipative treatment of Secs. II and III is generalized to include dissipation. In Sec. V we numerically evaluate the formula derived for the finite-temperature tunnel escape rate in the presence of (linear) dissipation. A conclusion follows Sec. V.

II. DENSITY MATRIX DESCRIBING THE METASTABLE STATE

In this section we set the foundations to our approach to tunneling. We derive the semiclassical approximation to the density matrix which describes the metastable state in the absence of dissipation. Consider a single particle with coordinate $q(t)$ moving in one dimension in a potential $V(q)$ which has a metastable minimum (Fig. 1).

We know that if the potential barrier is sufficiently high and wide, a particle initially trapped in the metastable minimum will behave to an excellent approximation as though the minimum is stable. In particular, if the particle is weakly coupled to a heat bath at temperature T it will come to a local thermal equilibrium at this temperature. The density matrix which approximately describes this metastable situation and does not include the extremely small currents associated with tunneling and classical escape processes is the object we shall derive next.

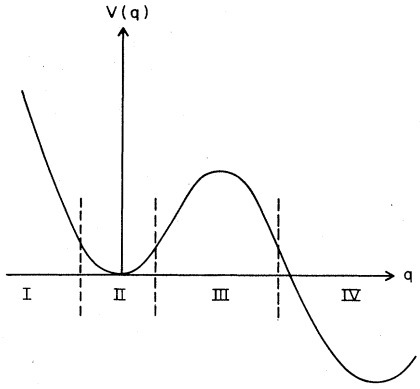

FIG. 1. A metastable potential.

The normalized density matrix of a particle with Hamiltonian

$$H=\frac{p^2}{2m}+V(q) \tag{2.1}$$

at temperature $T=\hbar/k_B\tau$ is given by

$$\rho(q,q';\tau)=\sum_n \psi_n(q)\psi_n^*(q')e^{-E_n\tau/\hbar}, \tag{2.2}$$

where $\psi_n(q)$ are the energy eigenfunctions of the Hamiltonian and E_n are the corresponding eigenvalues. This has a path-integral representation[29]

$$\rho(q,q';\tau)=\int_{q',=\tau/2}^{q,\tau/2} d[q]e^{-S[q]/\hbar}, \tag{2.3}$$

where

$$S[q]=\int_{-\tau/2}^{\tau/2} dt\left[\frac{m\dot{q}^2}{2}+V(q)\right] \tag{2.4}$$

and the notation of Eq. (2.3) means the functional integral over all trajectories starting at q' at "time" $-\tau/2$ and ending at q at time $\tau/2$.

The semiclassical approximation to Eq. (2.3) is summarized in Appendix A and the result is

$$\rho(q,q';\tau)\cong\sum_j N\det{}^{-1/2}[-m\partial_t^2+V''(\bar{q}_j(t))] \times\exp(-S[\bar{q}_j]/\hbar). \tag{2.5}$$

The trajectories $\bar{q}_j$ are classical trajectories in the *inverted* potential $-V(q)$ (Fig. 2) and satisfy equations (A5).

Let us reconsider the potential $V(q)$ of Fig. 1 which appears in Eq. (2.1). Note that we have included a second minimum of the potential. This reflects our expectation that in general there will be at least one minimum of the

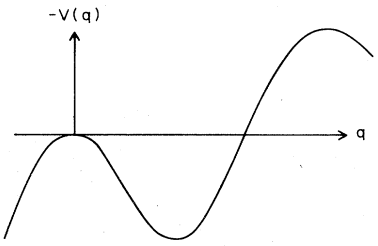

FIG. 2. The inverted metastable potential (of Fig. 1).

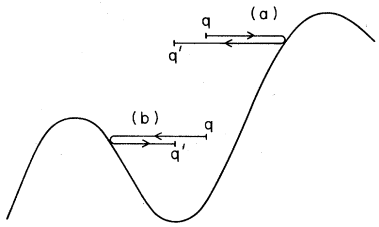

FIG. 3. Classical trajectories in the inverted potential from q to q' both with period τ.

potential other than the metastable minimum. There may be many more, but for the arguments we shall give a second minimum will be adequate. In order to avoid quantum coherence phenomena we shall always assume in what follows that the second minimum is far from being degenerate with the metastable minimum.

Let us return to the semiclassical approximation to the density matrix as given in Eq. (2.5). This contains the contributions of (in general) many classical trajectories $\{\bar{q}_j\}$ which move in the inverted potential (Fig. 2). The density matrix which describes the metastable state can be obtained by including in the sum of Eq. (2.5) the contribution from only a *single* trajectory.

This trajectory is determined by looking at a different density matrix, namely the density matrix for a pure harmonic potential $V_0(q)$ (the stable potential) which is centered on the origin (as is the metastable minimum) and has the same curvature as the metastable minimum at the origin. When the semiclassical approximation is made to the harmonic-oscillator density matrix a single trajectory will (exactly) dominate. Of the set of trajectories $\{\bar{q}_j\}$ appearing in Eq. (2.5) only a single one [say, $\bar{q}(t)$] will closely correspond to the trajectory dominating the harmonic-oscillator density matrix. It is $\bar{q}(t)$ when used in Eq. (2.5) which yields the density matrix of the metastable state.

A precise identification of $\bar{q}(t)$ may be made (if any ambiguity exists) by noting the following point. In the limit $q,q'\to 0$ a single trajectory $\bar{q}(t)$ out of the set $\{\bar{q}_j\}$ will exactly deform into the "harmonic-oscillator" trajectory (i.e., that trajectory dominating the harmonic-oscillator density matrix). This *uniquely* specifies $\bar{q}(t)$ and hence the density matrix computed from it. (We will subsequently consider values of q,q' which are not small.)

Let us make this clear with an example. If $q,q'>0$ and the time of motion, τ, is sufficiently large at least two classical trajectories in the inverted potential (Fig. 3) will be possible. (We draw the trajectories as horizontal lines at the energy of the motion.) To simplify Fig. 3 we have only included two classical trajectories; the omitted trajectories will play the same role as trajectory (a) in the ensuing reasoning. A comparison of these two trajectories and the trajectory in the inverted harmonic potential (Fig. 4) clearly shows that it is trajectory (b) of Fig. 3 which closely corresponds to the trajectory in the inverted harmonic potential.

The use of only the contribution of trajectory (b) in Eq. (2.5) yields the density matrix describing the metastable state (as we shall show below by comparison with the WKB result). Applying considerations such as the ones above, we obtain, for more general values of q,q' (but see later for limitations on these values), the following semiclassical approximation to the density matrix describing the metastable state:

$$\rho(q,q';\tau)=N\det{}^{-1/2}[-m\partial_t^2+V''(\bar{q}(t))]$$

$$\times\exp(-S[\bar{q}]/\hbar)\,, \tag{2.6}$$

where $\bar{q}$ is the appropriate "oscillatorlike" trajectory.

The statement that Eq. (2.6) is the semiclassical approximation to the density matrix which describes the metastable state will be elucidated shortly but let us note two points.

(1) Formula (2.6) for $\rho(q,q';\tau)$ certainly satisfies the boundary condition we would require of such an object, namely that for $q,q'\to 0$ it continuously deforms into the density matrix for the harmonic potential $V_0(q)$. This statement is in fact more restrictive than it need be. If, in the vicinity of the metastable minimum it is possible to write

$$V(q)=\frac{m\omega_0^2}{2}q^2(1-q/b)$$

then for $q,q'\ll b$, $\rho(q,q,';\tau)$ will be approximately that of a harmonic oscillator.

(2) The second point we note is that $\rho(q,q';\tau)$ is purely real and hence carries no current.

We can see the full content of the density matrix we have derived by obtaining the same quantity from WKB methods. To make the comparison easier we shall rewrite the functional determinant in Eq. (2.6) (Refs. 30 and 31) to obtain

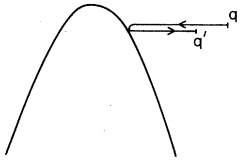

FIG. 4. The unique classical trajectory in the inverted oscillator potential from q to q' in time τ.

$$\rho(q,q';\tau)=\left[\frac{1}{2\pi\hbar}\frac{1}{|\dot{\bar{q}}(\tau/2)\dot{\bar{q}}(-\tau/2)|}\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|\right]^{1/2}$$

$$\times\exp(-S[\bar{q}]/\hbar)\,, \tag{2.7}$$

where $-E_{\rm cl}(q,q',\tau)$ is the energy of the motion in the inverted potential:

$$-E_{\rm cl}=\frac{m\dot{\bar{q}}^2}{2}-V(\bar{q})\,. \tag{2.8}$$

We shall now show how Eq. (2.7) arises from WKB methods.

In the potential of Fig. 1 we construct wave functions $\chi_n(q)$ with the following properties. In the classically accessible region II, $\chi_n(q)$ coincides with the normalized harmonic-oscillator energy eigenfunctions in the potential $V_0(q)$ which have energy $\epsilon_n=(n+\frac{1}{2})\hbar\omega_0$. In the classically forbidden regions I and III, $\chi_n(q)$ coincides with the spatially decaying WKB solutions (i.e.,

$$\chi_n(q)\sim\exp\left[-\frac{1}{\hbar}\int^{|q|}|p(q'\mathrm{sgn}(q))|\,dq'\right],$$

which smoothly join to the oscillator wave functions and are evaluated at energy ϵ_n).

It is the object

$$\rho(q,q';\tau)=\sum_n\chi_n(q)\chi_n(q')e^{-\epsilon_n\tau/\hbar}\,, \tag{2.9}$$

which corresponds to the density matrix of Eqs. (2.6) and (2.7).

To illustrate this we consider the specific case where q and q' lie in region III. In this region we have

$$\chi_n(q)=\frac{(mN_n)^{1/2}}{[\,|p_n(q)|\,]^{1/2}}\exp\left[-\frac{1}{\hbar}\int_{q_n}^{q}|p_n(q')|\,dq'\right] \tag{2.10}$$

with

$$p_n(q)=[2m(\epsilon_n-V(q))]^{1/2} \tag{2.11}$$

and q_n is defined by $p_n(q_n)=0$ $(q>q_n>0)$.

The factor N_n arises from the smooth joining to the oscillator wave functions. Use of Eq. (2.10) in Eq. (2.9) yields

$$\rho(q,q';\tau)=\sum_n\frac{N_n m}{[\,|p_n(q)p_n(q')|\,]^{1/2}}\exp\left[-\frac{1}{\hbar}\left[\int_{q_n}^{q}|p_n|\,dq''+\int_{q_n}^{q'}|p_n|\,dq''+\epsilon_n\tau\right]\right]. \tag{2.12}$$

The sum is converted to an integration over energy

$$\rho(q,q';\tau)=\int dE\frac{N(E)\rho(E)m}{\sqrt{|p(q,E)p(q',E)|}}\exp\left[-\frac{1}{\hbar}\left[\int_{q(E)}^{q}|p(E)|\,dq''+\int_{q(E)}^{q'}|p(E)|\,dq''+E\tau\right]\right], \tag{2.13}$$

where $\rho(E)$ is a density-of-states factor.

The integral is evaluated by making a Gaussian approximation to the integrand in which the extremum and quadratic fluctuations are determined solely by the exponent.

The extremum occurs at an energy $E_{\rm cl}$ which is the solution of

$$T_{\rm cl}(E_{\rm cl})=\tau\,, \tag{2.14}$$

where

$$T_{\rm cl}(E)=\int_{q(E)}^{q}\frac{m\,dq''}{|p(q'',E)|}+\int_{q(E)}^{q'}\frac{m\,dq''}{|p(q'',E)|}\,. \tag{2.15}$$

Equation (2.11) enables us to write

$$\frac{|p(q'',E_{\rm cl})|^2}{2m}-V(q'')=-E_{\rm cl}\,. \tag{2.16}$$

The velocity (parametrized by the position q''),

$$\dot{\bar{q}}(q'')\equiv\frac{|p(q'',E_{\rm cl})|}{m}\,, \tag{2.17}$$

corresponds to the motion (b) in the inverted potential depicted in Fig. 3. It follows that $\bar{q}(q'')$ is the same trajectory that appears in Eq. (2.6).

The Gaussian approximation to Eq. (2.13) is thus

$$\rho(q,q';\tau)=\frac{N(E_{\rm cl})\rho(E_{\rm cl})}{[\,|\dot{\bar{q}}(\tau/2)\dot{\bar{q}}(-\tau/2)|\,]^{1/2}}e^{-S[\bar{q}]/\hbar}\int_{-\infty}^{\infty}dE\exp-\frac{(E-E_{\rm cl})^2|T'_{\rm cl}(E_{\rm cl})|}{2\hbar}$$

$$=[2\pi\hbar N(E_{\rm cl})\rho(E_{\rm cl})]\left[\frac{1}{2\pi\hbar|\dot{\bar{q}}(\tau/2)\dot{\bar{q}}(-\tau/2)|}\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|\right]^{1/2}e^{-S[\bar{q}]/\hbar}\,, \tag{2.18}$$

where

$$S[\bar{q}]=\int_{q_{\rm cl}}^{q}m\dot{\bar{q}}(q'')dq''+\int_{q_{\rm cl}}^{q'}m\dot{\bar{q}}(q'')dq''+E_{\rm cl}\tau$$

$$=\int_{-\tau/2}^{\tau/2}\left[\frac{m\dot{\bar{q}}^2}{2}(t)+V(\bar{q}(t))\right]dt\,. \tag{2.19}$$

Equation (2.18) is to be compared with Eq. (2.7). We do not arrive at any inconsistencies if we assume the two results are identical. The factor $2\pi\hbar N(E_{\rm cl})\rho(E_{\rm cl})$ is thus identified as unity. This can be confirmed by considering q,q' in region II—the (approximately) harmonic region in which the Gaussian approximation may be considered ex-

act. We conclude this section with the comment that the Gaussian approximation automatically converts a WKB sum into an integral.

III. TUNNEL ESCAPE RATE IN THE ABSENCE OF DISSIPATION

In this section we show how to obtain the finite-temperature tunnel escape rate from the density matrix derived in the preceding section. In the WKB approximation the calculation of the tunnel escape rate of a particle in a metastable state with energy E may be carried out in the following way.

In the classically accessible region IV of Fig. 1 we specify an outgoing wave

$$\psi_{\rm IV}(q)=\frac{C}{\sqrt{p(q)}}\exp\left[\frac{i}{\hbar}\int_{q_2}^{q}(E)p(q')dq'+i\pi/4\right] \tag{3.1}$$

[$q_2(E)$ is the turning point between regions III and IV].

Using the WKB connection formulas[6] we obtain the wave function in the classically forbidden region III of Fig. 1:

$$\psi_{\rm III}(q)=\frac{C}{\sqrt{|p(q)|}}\left[e^{(1/\hbar)\int_q^{q(E)}|p|dq'}+\frac{i}{2}e^{-(1/\hbar)\int_q^{q(E)}|p|dq'}\right] . \tag{3.2}$$

In regions I and II we approximate the wave function by the function $\chi_n(q)$ defined previously: normalized harmonic-oscillator wave function in region II joined to the WKB solution of region I which vanishes as $q\to-\infty$. The coefficient C of $\psi_{\rm III}(q)$ is determined by matching the amplitude of $\psi_{\rm III}$ and the harmonic-oscillator wave function over a part of region III. In doing so we ignore the small imaginary part of $\psi_{\rm III}(q)$.

We can now compute the probability current in region III or region IV, they are the same. We find a current

$$\Gamma=\frac{|C|^2}{m} . \tag{3.3}$$

This current corresponds to the tunneling of particles out of the metastable well and Γ^{-1} is the average time spent in the potential well. We shall refer to Γ as the tunnel escape rate.

If we consider only the spatially decaying part of $\psi_{\rm III}(q)$, i.e., the part which goes as

$$\exp\left[-\frac{1}{\hbar}\int^{q}|p|dq'\right] ,$$

which is the real part of the wave function:

$$\chi(q)\equiv{\rm Re}\psi_{\rm III}(q)=\frac{C}{\sqrt{|p(q)|}}e^{(1/\hbar)\int_q^{q(E)}|p|dq'} , \tag{3.4}$$

and we define the velocity

$$\dot{\bar{q}}(q)\equiv\frac{|p(q)|}{m} , \tag{3.5}$$

we can write the tunnel escape rate as

$$\Gamma=\frac{|C|^2}{m}=\lim_{q\to q(E)-}\dot{\bar{q}}(q)|\chi(q)|^2 . \tag{3.6}$$

Now if we construct a probability density which consists only of *spatially decaying WKB wave functions* beneath the barrier, i.e.,

$$P(q)=|\chi(q)|^2 \ \text{(region III)} , \tag{3.7}$$

then Eq. (3.6) can be written as

$$\Gamma=\lim_{q\to q(E)-}\dot{\bar{q}}(q)P(q) . \tag{3.8}$$

This formula has a generalization to finite temperatures which will form the basis of our approach to finite-temperature tunneling.

Before we discuss this generalization let us note that if we keep the definitions of the wave functions ψ in regions I and II unaltered in the definition of the probability density, then $P(q)$ is approximately normalized to unity in the sense

$$\int_{-\infty}^{q_{\rm III}}P(q)dq\simeq 1 , \tag{3.9}$$

where $q_{\rm III}$ is a point deep in region III.

Returning to Eq. (3.8), the finite-temperature generalization of this is

$$\Gamma(\tau)=\lim_{q\to q_p(\tau)-}\dot{\bar{q}}(q,\tau)P(q,\tau) , \tag{3.10}$$

where $P(q,\tau)$ is a WKB approximation to the probability density (built out of spatially decaying WKB wave functions beneath the barrier) at temperature $T=\hbar/k_B\tau$ and $\dot{\bar{q}}(q,\tau)$ is an appropriate velocity function which vanishes at $q=q_p(\tau)$.

We have, of course, a candidate for $P(q,\tau)$, namely the probability density derived from the density matrix of Eq. (2.6). However, $\rho(q,q';\tau)$ is not normalized to unity. We shall normalize it in the sense of Eq. (3.9) by dividing the trace of the density matrix corresponding to the stable potential, namely the harmonic oscillator. For this potential we have

$$\rho_0(q,q;\tau)=N\det{}^{-1/2}[-m\partial_t^2+m\omega_0^2]e^{-q^2/2\langle q^2\rangle} , \tag{3.11}$$

where

$$\langle q^2\rangle=\frac{\hbar}{2m\omega_0}\coth\left[\frac{\omega_0\tau}{2}\right] . \tag{3.12}$$

Hence

$$P(q,\tau)=\frac{\rho(q,q;\tau)}{{\rm Tr}\rho_0} , \tag{3.13}$$

$$P(q,\tau)=\frac{1}{(2\pi\langle q^2\rangle)^{1/2}}\left[\frac{\det(-m\partial_t^2+V''(\bar{q}(t))}{\det(-m\partial_t^2+m\omega_0^2)}\right]^{-1/2}\times e^{-S[\bar{q}]/\hbar} . \tag{3.14}$$

In Fig. 5 we show the trajectory $\bar{q}(t)$ in the inverted potential. We assume $\omega\tau>2\pi$ where $-m\omega^2$ is the curvature of $V(q)$ at the top of the barrier (i.e., at q_0).

We note that if Eq. (3.10) [with $P(q,\tau)$ as given by Eq.

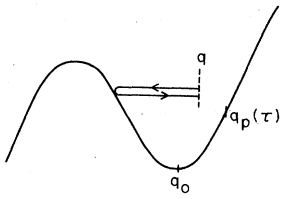

FIG. 5. A returning but nonperiodic classical trajectory in the inverted potential.

(3.14)] is to have a meaning, then for q in the vicinity of $q_p(\tau)$ (at which point $\bar{p}$ vanishes) $P(q,\tau)$ must be of the WKB form

$$P(q,\tau)=\frac{A(q,\tau)}{\dot{\bar{q}}(q;\tau)} \tag{3.15}$$

with $A(q,\tau)$ a function possessing a limiting value as $q\to q_p(\tau)-$.

If we consider the motion of Fig. 5, it is evident that the largest value of the end point q that can be specified for the prescribed trajectory to exist is $q=q_p(\tau)$ at which point the end point is a turning point of the motion. As is well known, many quantities of classical mechanics are singular in the vicinity of a turning point and for the above probability density [Eq. (3.14)] the singularity manifests itself in the lowest two eigenvalues of the functional determinant

$$N^{-2}\det[-m\partial_t^2+V''(\bar{q}(t))] .$$

It is very natural to expect the behavior of Eq. (3.15) to arise from these two eigenvalues and hence we shall investigate their behavior as a function of q at fixed τ.

The operator $-m\partial_t^2+V''(\bar{q}(t))$ is analogous to the Hamiltonian operator in the Schrodinger equation where the role of the coordinate is played by the time t. We shall always imagine the potential $V(q)$ to be of the form

$$V(q)=\frac{m\omega_0^2}{2}q^2(1-q/b) ; \tag{3.16}$$

however, the conclusions we come to will be of more general validity.

We use the following procedure to obtain detailed information on the lowest two eigenvalues of the Schrodinger operator. The eigenvalue equation is [Eq. (A15)]

$$[-m\partial_t^2+V''(\bar{q}(t))]\phi_n(t)=\lambda_n\phi_n(t) \tag{3.17}$$

with boundary conditions

$$\phi_n(\pm\tau/2)=0 . \tag{3.18}$$

The equation of motion which $\bar{q}(t)$ satisfies is [Eq. (A6)]

$$-m\ddot{\bar{q}}(t)+V'(\bar{q}(t))=0 . \tag{3.19}$$

The time derivative of this is

$$[-m\partial_t^2+V''(\bar{q}(t))]\dot{\bar{q}}(t)=0 . \tag{3.20}$$

We note that $\dot{\bar{q}}(t)$ is an antisymmetric function with a single node. When $\dot{\bar{q}}(\pm\tau/2)=0$, $\dot{\bar{q}}(t)$ satisfies both the eigenvalue equation [Eq. (3.17)] and the boundary conditions [Eq. (3.18)]. Thus *only* when $\dot{\bar{q}}(\pm\tau/2)=0$ is $\dot{\bar{q}}$ an eigenfunction of Eq. (3.17) with the correct boundary behavior. The antisymmetric eigenfunction associated with the second smallest eigenvalue, $\phi_2(t)$, is similar to $\dot{\bar{q}}(t)$ in that it has a single node. It is clear that when $\dot{\bar{q}}(\pm\tau/2)\to 0$, $\dot{\bar{q}}(t)$ must (within a normalization) become $\phi_2(t)$.

Accordingly, for small $\dot{\bar{q}}(\pm\tau/2)$ it is a good approximation to write

$$\phi_2(t)=\frac{\dot{\bar{q}}(t)}{||\dot{\bar{q}}||} , \tag{3.21}$$

where

$$||\dot{\bar{q}}||\equiv\left[\int_{-\tau/2}^{\tau/2}\dot{\bar{q}}^2(t)dt\right]^{1/2} \tag{3.22}$$

ensures the approximation to $\phi_2(t)$ is correctly normalized to unity.

Let us now form the following quantity. For $n=2$ multiply Eq. (3.17) by $\dot{\bar{q}}(t)$ and subtract Eq. (3.19) multiplied by $\phi_2(t)$. We obtain

$$-m[\dot{\bar{q}}(t)\partial_t^2\phi_2(t)-\phi_2(t)\partial_t^2\dot{\bar{q}}(t)]=\lambda_2\phi_2(t)\dot{\bar{q}}(t) . \tag{3.23}$$

Integrating this form 0 to $\tau/2$ and using $\phi_2(\tau/2)=\phi_2(0)=\dot{\bar{q}}(0)=0$, we obtain

$$-m\dot{\bar{q}}(\tau/2)\dot{\phi}_2(\tau/2)=\lambda_2\int_0^{\tau/2}dt\,\phi_2(t)\dot{\bar{q}}(t) . \tag{3.24}$$

Use of the approximation Eq. (3.21) in Eq. (3.24) gives

$$\lambda_2\simeq\frac{2m\,|\ddot{\bar{q}}(\tau/2)|}{||\dot{\bar{q}}||^2}\dot{\bar{q}}(\tau/2) \tag{3.25}$$

(we have used the fact that $\ddot{\bar{q}}(\tau/2)<0$). Equation (3.25) reveals the way λ_2 vanishes as the end-point velocity becomes small.

Let us now use a similar method to find the lowest eigenvalue λ_1—belonging to the symmetric eigenfunction $\phi_1(t)$. We go back to Eq. (3.17), set $n=2$, multiply by $\phi_1(t)$, and subtract the corresponding quantity with $2\rightleftarrows 1$. Integrating this from 0 to $\tau/2$, we quickly find for small $\dot{\bar{q}}(\tau/2)$

$$\lambda_1\simeq\frac{2m\,|\ddot{\bar{q}}(\tau/2)|}{||\dot{\bar{q}}||}[\dot{\bar{q}}(\tau/2)-\Delta] , \tag{3.26}$$

where

$$\Delta\equiv\frac{||\dot{\bar{q}}||^2}{|\bar{q}(\tau/2)|}\frac{\phi_1(0)\dot{\phi}_2(0)}{2\int_0^{\tau/2}dt\,\phi_1(t)\phi_2(t)} . \tag{3.27}$$

From the behavior of ϕ_1 and ϕ_2 it immediately follows that $\Delta\geq 0$. (We have found $\Delta=0$ only for $\tau=\infty$.) The implications of Eqs. (3.26) and (3.27) are that $P(q,\tau)$ does *not* behave as in Eq. (3.15), but rather

$$P(q,\tau)\propto\frac{1}{(\lambda_1\lambda_2)^{1/2}}\propto\frac{1}{[\dot{\bar{q}}(\tau/2)[\dot{\bar{q}}(\tau/2)-\Delta]]^{1/2}} . \tag{3.28}$$

This is at first sight a surprising result. It means $P(q,\tau)$ does not diverge in a WKB manner (i.e., as the inverse of the velocity) at $q=q_p(\tau)$, but because of the presence of Δ it diverges at a value of q *smaller* than $q_p(\tau)$.

In order to understand the behavior in Eq. (3.28) let us first note that Eq. (2.7) gives a representation of $\rho(q,q';\tau)$ which results on setting $q'=q$, in

$$P(q,\tau)\propto\rho(q,q,\tau)\propto\frac{1}{\dot{\bar{q}}(\tau/2)}\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|^{1/2}. \tag{3.29}$$

Equations (3.28) and (3.29) can be reconciled to one another if

$$\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|\propto\left[\frac{\dot{\bar{q}}(\tau/2)}{\dot{\bar{q}}(\tau/2)-\Delta}\right]. \tag{3.30}$$

In Appendix B we show that this is indeed the case. The anomalous behavior $[\dot{\bar{q}}(\tau/2)-\Delta]^{-1/2}$ is therefore directly attributable to the factor $|\partial E_{\rm cl}/\partial\tau|^{1/2}$, which from Eq. (2.18) can be seen to arise from quadratic energy fluctuations about $E_{\rm cl}$. Thus for q in the vicinity of $q_p(\tau)$ the Gaussian approximation as used in Eq. (2.18) is breaking down.

The resolution of the problem is to repeat the derivation leading to Eq. (2.18) this time using the "exact" wave functions in the vicinity of $q=q_p(\tau)$. These are, of course, Airy functions. The calculation is straightforward and we find for q extremely close to $q_p(\tau)$, *inter alia,* the factor $|\partial E_{\rm cl}/\partial\tau|^{1/2}$ is replaced by $|\partial E_p/\partial\tau|^{1/2}$ where $-E_p$ is the energy of the periodic motion in the inverted potential (i.e., the motion starts and ends at $q_p(\tau)$ and takes a time τ to do so). Thus to correct the quadratic energy fluctuations for q close to $q_p(\tau)$ we make the replacement

$$\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|^{1/2}\rightarrow\left|\frac{\partial E_p}{\partial\tau}\right|^{1/2}. \tag{3.31}$$

However, from Eq. (B14) we have

$$\left|\frac{\partial E_p}{\partial\tau}\right|^{1/2}\cong\left[\frac{\dot{\bar{q}}(\tau/2)-\Delta}{\dot{\bar{q}}(\tau/2)}\right]^{1/2}\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|^{1/2}, \tag{3.32}$$

hence Eq. (3.31) can be written as

$$\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|^{1/2}\rightarrow\left[\frac{\dot{\bar{q}}(\tau/2)-\Delta}{\dot{\bar{q}}(\tau/2)}\right]^{1/2}\left|\frac{\partial E_{\rm cl}}{\partial\tau}\right|^{1/2} \tag{3.33}$$

which is a simple multiplicative correction.

The probability density corresponding to Eq. (3.14) but with the *corrected* quadratic energy fluctuations is, by virtue of the implicit $|\partial E_{\rm cl}/\partial\tau|^{1/2}$ factor,

$$\bar{P}(q,\tau)\equiv\left[\frac{\dot{\bar{q}}(\tau/2)-\Delta}{\dot{\bar{q}}(\tau/2)}\right]^{1/2}P(q,\tau) \tag{3.34}$$

and using Eq. (3.28) we see that

$$\bar{P}(q,\tau)\propto\frac{1}{\dot{\bar{q}}(\tau/2)}. \tag{3.35}$$

On account of the $\dot{\bar{q}}(\tau/2)^{-1}$ factor, $\bar{P}(q,\tau)$ is of manifestly WKB form and is the correct probability density to use in Eq. (3.10) for the finite-temperature tunnel escape rate.

We have

$$\Gamma(\tau)=\lim_{q\rightarrow q_p(\tau)-}\dot{\bar{q}}(q,\tau)\bar{P}(q,\tau), \tag{3.36}$$

and using Eqs. (3.14), (3.25), (3.27), and (3.34) we obtain [this result may be shown to be equivalent to Eq. (9) of Ref. 7; it follows directly from Eqs. (2.18), (3.13), (3.32), (3.34), and (3.36)]:

$$\Gamma(\tau)=\frac{1}{(2\pi\langle q^2\rangle)^{1/2}}\frac{\|\dot{\bar{q}}\|^2}{2m\,|\ddot{\bar{q}}(\tau/2)|}\times\left[\frac{\det''(-m\partial_t^2+V''(\bar{q}(t)))}{\det(-m\partial_t^2+m\omega_0^2)}\right]^{-1/2}e^{-S[\bar{q}]/\hbar}, \tag{3.37}$$

where the double prime on the determinant denotes the omission of the lowest two eigenvalues.

For the potential

$$V(q)=\frac{m\omega_0^2}{2}q^2\left[1-\frac{q}{b}\right]$$

and in the zero-temperature limit, it is possible to analytically evaluate Eq. (3.37). We find

$$\Gamma_0=\omega_0\left[\frac{30S_0}{\pi\hbar}\right]^{1/2}e^{-S_0/\hbar},\qquad S_0=\frac{16}{15}\frac{m\omega_0^2b^2}{2}, \tag{3.38}$$

which is identical with the ground-state WKB result. We shall conclude this section with some comments on the formula (3.37) for the tunneling rate.

A. Number of metastable states

In the derivation of the tunneling-rate formula we did not make any assumptions about the number of metastable states bound in the potential well, but we did make the semiclassical approximation to the density matrix. In principle, it should be possible to determine (from an examination of the semiclassical approximation) the minimum number of metastable states required for validity of Eq. (3.37); at present, however, this is still an open problem. We should note that in order to have a tunneling rate which is temperature dependent [which always follows from Eq. (3.37)] it is necessary to have at least two metastable states within the potential well.

B. Maximum temperature of validity

The periodic orbit used in Eq. (3.37) corresponds to tunneling being concentrated about the horizontal line shown in Fig. 6 which lies at energy E_p. As the temperature is increased, E_p increases and the horizontal line

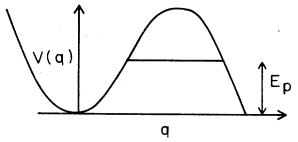

FIG. 6. The line about which tunneling is concentrated in the metastable potential.

moves up. This eventually takes us into a small region near the top of the barrier where the linear WKB turning-point formulas break down. If the curvature at the top of the barrier is denoted by $-m\omega^2$, then the breakdown occurs at temperatures close to, but less than, $T=\hbar\omega/2\pi k_B$ (i.e., $\omega\tau=2\pi$). Such behavior has been discussed in Ref. 7 and interpreted as the crossover from quantum to classical escape processes. The formula for $\Gamma(\tau)$ will be valid outside this region (i.e., lower temperatures) but it is a delicate problem to specify the precise temperature at which it ceases to be valid.

Let us note that in the formula of Eq. (3.37) the exponent $S[\bar{q}]/\hbar$ has the value βV_0 for $k_BT>\hbar\omega/2\pi$, where $\beta=1/k_BT$ and V_0 is the height of the barrier. This is the exponent of the classical activation process (Ref. 1). It is therefore natural to assume that $S[\bar{q}]/h$ is the correct escape-rate exponent for *all* temperatures.

Unlike the exponent, the prefactor in (4.2) (i.e., the quantity multiplying $e^{-S/\hbar}$) cannot be used in the vicinity of $k_BT=\hbar\omega/2\pi$ with meaningful results. This is because at the temperature $T=\hbar\omega/2\pi k_B$ ($\omega\tau=2\pi$) the factor $||\dot{\bar{q}}||^2/|\ddot{\bar{q}}(\tau/2)|$ vanishes and so does the prefactor.

C. Generalization to include dissipation

Let us remark that the reason why we convert the (simpler) Eq. (2.18) into the (more complicated) Eq. (3.37) is that the former has no obvious generalization to the dissipative case.

IV. TUNNEL ESCAPE RATE IN THE PRESENCE OF DISSIPATION

In the preceding section we calculated the finite-temperature tunnel escape rate in the absence of dissipation. In the calculation the central role was played by the approximate wave functions in the probability density and not the energy levels of the metastable system. This emphasis will, as we shall see in this section, enable us to apply a similar procedure in the case where dissipation is present.

The problem we avoid by not concentrating on energy levels is that they are quite different in the dissipative and nondissipative cases. In particular, in the dissipative case the metastable system must be viewed as part of a larger system—the metastable system and its environment—which has a continuous set of energy levels.

In order to incorporate dissipation into the finite-temperature tunneling calculation we use a model of dissipation formulated by Caldeira and Leggett.[11] This employs the Lagrangian

$$L=\frac{m\dot{q}^2}{2}-V(q)+\sum_\alpha\left[\frac{m_\alpha\dot{x}_\alpha^2}{2}-\frac{m_\alpha\omega_\alpha^2x_\alpha^2}{2}\right]-q\sum_\alpha c_\alpha x_\alpha-\tfrac{1}{2}q^2\sum_\alpha\frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\,. \tag{4.1}$$

The coordinate q represents the variable of the system of interest (the tunneling variable), we shall call it the "particle." The variables $\{x_\alpha\}$ denote the degrees of freedom of the environment and the coupling between the particle and the environment is governed by the constants $\{c_\alpha\}$. A detailed justification of the above Lagrangian as a description of linear dissipation has been given in Ref. 11 for the case of zero temperature; we shall assume it has validity at nonzero temperatures.

All information on the environment of relevance to the particle is contained in the spectral density

$$J(\omega)=\frac{\pi}{2}\sum_\alpha\frac{c_\alpha^2}{m_\alpha\omega_\alpha}\delta(\omega-\omega_\alpha)\,. \tag{4.2}$$

If

$$J(\omega)=\eta\omega \tag{4.3}$$

it can be shown[11] that the classical equation of motion which q obeys is (at zero temperature)

$$m\ddot{q}+\eta\dot{q}=-\frac{dV(q)}{dq}\,. \tag{4.4}$$

Hence η in Eq. (4.3) corresponds to the friction constant of the classical motion of the particle and can be experimentally determined.

We shall limit ourselves to the linear spectral density of Eq. (4.3); however, it is probable that the methods we shall adopt apply to more general spectral densities.

The procedure we use to obtain the tunneling rate in the presence of dissipation takes the following form. We investigate the behavior of the approximate probability density which describes the metastable state. We take the signature of tunneling to be the appearance of a velocity denominator which is characteristic of WKB wave function. The probability current is then assumed (this assumption has been considered in some detail in Ref. 24) to be given by the same formula as in the undamped case.

Let us now make an explicit statement of our objective. We have a particle (or more generally a system) with coordinate q subject to dissipation as described by Eqs. (4.1), (4.2), and (4.3). It is known that initially the particle is localized in a metastable minimum of the potential. We assume the particle comes to a local thermal equilibrium at the temperature $T=\hbar/k_B\tau$ of the oscillator environment. Our objective is to determine the rate of the tunneling of the particle out of the metastable minimum. The calculation of the tunneling rate now follows.

We first have to obtain the density matrix describing the metastable state. The complete density matrix describing the particle and the environment at temperature $T=\hbar/k_B\tau$ is given (Ref. 11, Sec. IV) by

$$\rho(q\{x_\alpha\},q'\{x'_\alpha\},\tau)$$
$$=\sum_r \psi_n(q\{x_\alpha\})\psi_n(q'\{x'_\alpha\})e^{-E_n\tau/\hbar} \tag{4.5}$$
$$=\int_{q'\{x'_\alpha\},-\tau/2}^{q\{x_\alpha\},\tau/2} \prod_\alpha d[x_\alpha]d[q]e^{-\bar{S}[q\{x_\alpha\}]/\hbar} . \tag{4.6}$$

In Eq. (4.5) $\psi_n(q\{x_\alpha\})$ are the eigenfunctions of the quantum-mechanical Hamiltonian derived from the Lagrangian of Eq. (4.1) and the E_n are the corresponding eigenvalues. In Eq. (4.6)

$$\bar{S}[q\{x_\alpha\}]=\int_{-\tau/2}^{\tau/2}dt\left[\frac{m\dot{q}^2}{2}+V(q)+\sum_\alpha\frac{m_\alpha x_\alpha^2}{2}+\frac{m_\alpha\omega_\alpha^2x_\alpha^2}{2}+qc_\alpha x_\alpha+q^2\frac{c_\alpha^2}{2m_\alpha\omega_\alpha^2}\right] . \tag{4.7}$$

Provided we only compute currents of the particle and make no specifications on the state of the environment, the appropriate density matrix is not the full density matrix but rather the *reduced* density matrix obtained by tracing out the environment. The reduced density matrix is defined by

$$\rho(q,q',\tau)\equiv\frac{\int_{-\infty}^{\infty}\prod_\alpha dx_\alpha\rho(q\{x_\alpha\},q'\{x_\alpha\};\tau)}{\prod_\alpha[2\sinh(\omega_\alpha\tau/2)]^{-1}} . \tag{4.8}$$

Following Ref. 11 we perform the x_α integrations (in this work we do not periodically continue the trajectory unlike Ref. 11) to obtain

$$\rho(q,q';\tau)=\int_{q',-\tau/2}^{q,\tau/2}d[q]e^{-S[q]/\hbar} , \tag{4.9}$$

where

$$S[q]=\int_{-\tau/2}^{\tau/2}dt\left[\frac{mq^2}{2}+V(q)\right]+\frac{\eta\pi}{4\tau^2}\int_{-\tau/2}^{\tau/2}ds\int_{-\tau/2}^{\tau/2}dt\left[\frac{q(t)-q(s)}{\sin\left[\frac{\pi(t-s)}{\tau}\right]}\right]^2 . \tag{4.10}$$

The semiclassical approximation to the reduced density matrix may be obtained by using the methods of Appendix A. We find

$$\rho(q,q',\tau)=\sum_j N\det{}^{-1/2}[-m\partial_t^2+V''(\bar{q}_j(t))+\hat{O}_t]\times e^{-S[\bar{q}_j]/\hbar} , \tag{4.11}$$

where the integral operator $\hat{O}_t$ is defined by

$$\hat{O}_t\phi(t)=\frac{\eta\pi}{\tau^2}\int_{-\tau/2}^{\tau/2}ds\frac{\phi(t)-\phi(s)}{\sin^2\left[\frac{\pi(t-s)}{\tau}\right]} \tag{4.12}$$

and each extremal trajectory satisfies

$$\bar{q}(-\tau/2)=q',\ \bar{q}(\tau/2)=q ,$$
$$-m\ddot{\bar{q}}(t)+V'(\bar{q}(t))+\hat{O}_t q(t)=0 . \tag{4.13}$$

The density matrix for the metastable state in the presence of dissipation now results from Eq. (4.11) by the same considerations we gave in Sec. II for the undamped case. That is, out of the set of extremal trajectories $\{q_j\}$ in Eq. (4.11) we select the single trajectory $\bar{q}$ corresponding most closely to the trajectory determining the reduced density matrix of the (damped) harmonic oscillator. The contribution of $\bar{q}$ in Eq. (4.11) results in the required density matrix:

$$\rho(q,q';\tau)=N\det{}^{-1/2}[-m\partial_t^2+V''(\bar{q}(t))+\hat{O}_t]e^{-S[\bar{q}]/\hbar} . \tag{4.14}$$

The normalized probability density is given by

$$P(q,\tau)=\frac{\rho(q,q;\tau)}{\mathrm{Tr}\rho_0} , \tag{4.15}$$

where ρ_0 is the density matrix for the damped harmonic oscillator. In Appendix C we show that the diagonal elements of ρ_0 are

$$\rho_0(q,q;\tau)=N\det{}^{-1/2}(-m\partial_t^2+m\omega_0^2+\hat{O}_t)e^{-q^2/2\langle q^2\rangle} , \tag{4.16}$$

where

$$\langle q^2\rangle=\frac{\hbar}{m\pi}\int_0^\infty d\omega\coth\left[\frac{\omega\tau}{2}\right]\frac{2\gamma\omega}{(\omega_0^2-\omega^2)^2+(2\gamma\omega)^2} . \tag{4.17}$$

Hence Eqs. (4.14)—(4.16) give, on evaluating the trace, the probability density

$$P(q,\tau)=\frac{1}{(2\pi\langle q^2\rangle)^{1/2}}\left[\frac{\det[-m\partial_t^2+V''(\bar{q}(t))+\hat{O}_t]}{\det(-m\partial_t^2+m\omega_0^2+\hat{O}_t)}\right]^{-1/2}\times e^{-S[\bar{q}]/\hbar} . \tag{4.18}$$

In order to investigate the behavior of the lowest two eigenvalues of the anharmonic determinant (i.e., $\det[-m\partial_t^2+V''(\bar{q}(t))+\hat{O}_t]$) we introduce the notation

$$K(s-t)\equiv\frac{\eta\tau}{\tau^2}\frac{1}{\sin^2\left[\frac{\pi(t-s)}{\tau}\right]} . \tag{4.19}$$

The eigenvalue equation (for each of the eigenvalues of the anharmonic determinant) is

$$[-m\partial_t^2+V''(\bar{q}(t))]\phi_n(t)+\int_{-\tau/2}^{\tau/2}ds\,K(s-t)[\phi_n(t)-\phi_n(s)]=\lambda_n\phi_n(t) \tag{4.20}$$

and the time derivative of the classical equation of motion [Eq. (4.13)] is

$$[-m\partial_t^2+V''(\bar{q}(t))]\dot{\bar{q}}(t) + \int_{-\tau/2}^{\tau/2} ds\, K(s-t)[\dot{\bar{q}}(t)-\dot{\bar{q}}(s)]=0 . \quad (4.21)$$

If we repeat the steps following Eq. (3.20) that led to equations (3.25) and (3.26), but this time using the above two equations, we find on using symmetry of $K(s)$ and antisymmetry of $\phi_2(s)$ that the lowest two eigenvalues for small $\dot{\bar{q}}(\tau/2)$ are given by

$$\lambda_1 \cong \frac{2m\,|\ddot{\bar{q}}(\tau/2)|}{||\dot{\bar{q}}||^2}\dot{\bar{q}}(\tau/2) , \quad (4.22)$$

$$\lambda_2 \cong \frac{2m\,|\ddot{\bar{q}}(\tau/2)|}{||\dot{\bar{q}}||^2}[\dot{\bar{q}}(\tau/2)-\Delta] , \quad (4.23)$$

where

$$\Delta=\frac{||\dot{\bar{q}}||^2}{2m\,|\bar{q}(\tau/2)|}\frac{m\phi_1(0)\dot{\phi}_2(0)+2\int_0^{\tau/2}ds\int_0^{\tau/2}dr\,K(s+t)\phi_1(s)\phi_2(t)}{\int_0^{\tau/2}dt\,\phi_1(t)\phi_2(t)} . \quad (4.24)$$

We see, therefore, that λ_1 and λ_2 take the same form as in the nondissipative case (however, Δ has a modified structure). Hence Eq. (3.28) still describes the behavior of the probability density when $\dot{\bar{q}}(\tau/2)$ is small.

In the nondissipative case the origin of the $(\dot{\bar{q}}-\Delta)^{1/2}$ factor was explicitly known—it arose from the breakdown in quadratic energy fluctuations when the end-point velocity was small. The different quadratic part of the action of the dissipative system has resulted in Δ having a modified structure; however, the underlying origins of this factor must be the same. We therefore make the assumption that the way to correct these quadratic fluctuations in the dissipative case takes precisely the same form as in the nondissipative case, namely multiply $P(q,\tau)$ by the factor

$$\left[\frac{\dot{\bar{q}}(\tau/2)-\Delta}{\dot{\bar{q}}(\tau/2)}\right]^{1/2} , \quad (4.25)$$

where $\dot{\bar{q}}(\tau/2)$ and Δ are appropriate to the dissipative case.

The probability density with the corrected quadratic fluctuations is

$$\bar{P}(q,\tau)\equiv\left[\frac{\dot{\bar{q}}(\tau/2)-\Delta}{\dot{\bar{q}}(\tau/2)}\right]^{1/2}P(q,\tau) . \quad (4.26)$$

We find

$$\bar{P}(q,\tau)=\frac{1}{\dot{\bar{q}}(q)}\frac{||\dot{\bar{q}}||^2}{2m\,|\ddot{\bar{q}}(\tau/2)|}\times\left[\frac{\det''[-m\partial_t^2+V''(\bar{q}(t))+\hat{O}_t]}{\det(-m\partial_t^2+m\omega_0^2+\hat{O}_t)}\right]^{1/2}\times e^{-S[\bar{q}]/\hbar} . \quad (4.27)$$

In the absence of dissipation, the tunnel escape rate (i.e., the probability current beneath the barrier) was given by

$$\Gamma(\tau)=\lim_{q\to q_p(\tau)-}\dot{\bar{q}}(q,\tau)\bar{P}(q,\tau) \quad (4.28)$$

in which $\bar{P}(q,\tau)$ was constructed out of WKB wave functions.

In the dissipative case we have a probability density Eq. (4.27) which possesses a factor $\dot{\bar{q}}(q)^{-1}$. This factor indicates that the probability density is constructed out of WKB wave functions of which $\dot{\bar{q}}(q)$ is characteristic of the "average" wave functions. [A decomposition of $P(q,\tau)$ into the form:

$$P(q,\tau)=\sum C_{nm}\psi_n^*(q)\psi_m(q)$$

is always possible.] We make, therefore, the natural conjecture that Eq. (4.28) generalizes to give the tunnel escape rate in the presence of dissipation. Making use of the above conjecture we use Eq. (4.27) in Eq. (4.28) to obtain the finite-temperature tunnel escape rate in the presence of dissipation:

$$\Gamma(\tau)=\frac{1}{(2\pi\langle q^2\rangle)^{1/2}}\frac{||\dot{\bar{q}}||^2}{2m\,|\ddot{\bar{q}}(\tau/2)|}\times\left[\frac{\det''[-m\partial_t^2+V''(\bar{q}(t))+\hat{O}_t]}{\det(-m\partial_t^2+m\omega_0^2+\hat{O}_t)}\right]^{-1/2}\times e^{-S[\bar{q}]/\hbar} , \quad (4.29)$$

where $S[\bar{q}]$ is given by Eq. (4.10) and all quantities are evaluated on the trajectory in which $\dot{\bar{q}}(\tau/2)=0$.

The formula (4.29) is the main result of this paper. Let us note that the exponent of the tunnel-escape-rate formula of Eq. (4.29) $S[\bar{q}]/\hbar$ coincides with the action found by Caldeira and Leggett[11] in the zero-temperature limit. For finite temperature it coincides with the result found in Ref. 21.

We also note that with similar behavior to the nondissipative case, the exponent achieves the classical activation rate βV_0 at sufficiently high temperatures and we shall assume that $S[\bar{q}]/\hbar$ is the correct escape-rate exponent for all temperatures.

V. NUMERICAL EVALUATION OF THE TUNNEL-ESCAPE-RATE FORMULA

The result obtained for the finite-temperature tunnel escape rate in the presence of dissipation has the form $Ae^{-S/\hbar}$ where A is termed the prefactor and S the action. The tunneling rate depends sensitively on the action and relatively insensitively on the prefactor. In this section we shall fairly precisely evaluate the action and approximately evaluate the prefactor. The potential we consider is the case of practical interest; quadratic plus cubic.

First we evaluate the action. The action $S[q]$ in the escape-rate formula is given by Eq. (4.10). We write the potential appearing in this as

$$V(q)=\frac{m\omega_0^2}{2}q^2(1-q/b)\ . \tag{5.1}$$

The distance b is the width of the barrier.

$V(q)$ has a maximum at $q=2b/3$ and the height of the potential barrier [with respect to $V(q=0)$] is

$$V_0\equiv V(2b/3)=\frac{4}{27}\frac{m\omega_0^2b^2}{2}\ . \tag{5.2}$$

Let us introduce some dimensionless quantities

$$u\equiv\omega_0 t,\quad v\equiv\omega_0 s\ , \tag{5.3}$$

$$\Omega\equiv\omega_0\tau=\frac{\hbar\omega_0}{k_BT}\ , \tag{5.4}$$

$$Z(u)\equiv\bar{q}(t)/b\ , \tag{5.5}$$

$$\alpha\equiv\eta/2m\omega_0\ , \tag{5.6}$$

$$\sigma[Z]\equiv(S[\bar{q}]/\hbar)\Big/\frac{m\omega_0b^2}{2\hbar}\ , \tag{5.7}$$

The dimensionless action of Eq. (5.7) can be written as

$$\sigma[Z]=\int_{-\Omega/2}^{\Omega/2}du[Z'(u)^2+Z(u)^2-Z(u)^3]+\frac{\alpha}{\pi}\int_{-\Omega/2}^{\Omega/2}du\int_{-\Omega/2}^{\Omega/2}dv\left[\frac{Z(u)-Z(v)}{\frac{\Omega}{\pi}\sin\left[\frac{\pi(u-v)}{\Omega}\right]}\right]^2. \tag{5.8}$$

Since $\bar{q}(t)$ is an extremum of $S[q]$, it follows that $Z(u)$ is an extremum of $\sigma[Z]$. Hence $Z(u)$ obeys the equation of motion

$$-Z''(u)+Z(u)-\frac{3Z^2}{2}(u)+\frac{2\alpha}{\pi}\int_{-\Omega/2}^{\Omega/2}dv\frac{Z(u)-Z(v)}{\left[\frac{\Omega}{\pi}\sin\left[\frac{\pi(u-v)}{\Omega}\right]\right]^2}=0\ . \tag{5.9}$$

Chang and Chakravarty (Ref. 17, Sec. III) solved this equation for the case $\Omega=\infty$, $Z(\pm\infty)=0$, and hence obtained the action $\sigma[Z]$. By a generalization of their procedure we have solved Eq. (5.9) for the case of finite Ω (i.e., nonzero temperature) with boundary conditions upon $Z(u)$ appropriate to our case:

$$Z(-\Omega/2)=Z(\Omega/2),\quad \max_u Z(u)=Z(\Omega/2)\ . \tag{5.10}$$

The generalization consists of replacing Fourier integrals by Fourier sums and using a different choice of starting function. The procedure is as follows: $Z(u)$ is represented as a Fourier sum

$$Z(u)=\sum_{n=-\infty}^{\infty}Z_ne^{i\omega_nu},\quad \omega_n=\frac{2\pi n}{\Omega}\ . \tag{5.11}$$

The equation of motion (5.9) can be written in terms of the Fourier components $\{Z_n\}$ as

$$Z_n=\frac{3/2}{(\omega_n^2+2\alpha|\omega_n|+1)}\sum_p Z_pZ_{n-p}\ . \tag{5.12}$$

We introduce an operation $O_n(\lambda,Z)$ defined by

$$O_n(\lambda,Z)\equiv\frac{\lambda}{(\omega_n^2+2\alpha|\omega_n|+1)}\sum_p Z_pZ_{n-p}\ . \tag{5.13}$$

The discretized iteration procedure equivalent to that of Ref. 17 is (1) start with an initial function with Fourier components $\{Z_n^{(0)}\}$ and an initial choice of λ, λ_0; (2) calculate $Z_n^{(1)}=O_n(\lambda_0,Z^{(0)})\forall n$; (3) calculate $\lambda_1=\lambda_0/\xi^2$ where $\xi=Z_0^{(1)}/Z_0^{(0)}$; (4) find $Z_n^{(2)}=O_n(\lambda_1,Z^{(1)})\forall n$; (5) repeat steps (2)—(4) until a convergence criterion is met.

This procedure yields the set of numbers λ_N, $\{Z_n^{(N)}\}$, where N is the number of iterations. The Fourier components of the solution of Eq. (5.9) are given by

$$Z_n=\frac{2\lambda_N}{3}Z_n^{(N)}\ , \tag{5.14}$$

and in terms of these the action is

$$\sigma[Z]=\Omega\left[\sum_n Z_n^2(\omega_n^2+2\alpha|\omega_n|+1)-\sum_{nm}Z_mZ_nZ_{m+n}\right]. \tag{5.15}$$

The functions with which we started the iteration procedure were of the qualitative form shown in Fig. 7. In the evaluation of the operation O_n we truncated the sums at $n=50$ or 100 (this is of course determined by the temperature, low temperatures require a larger number of terms). By comparison with known results, we estimate the error in the action over the range of temperatures we consider to be smaller than 0.1%.

Let us now consider the temperature range over which the tunneling-rate formula Eq. (4.29) is valid. In the nondissipative case the corresponding formula became invalid when temperatures were sufficiently high that tunneling was principally occurring close to the top of the barrier.

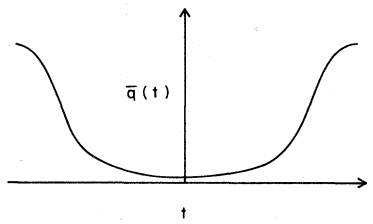

FIG. 7. The trajectory of Fig. 5 as a function of time.

TABLE I. Dimensionless cross-over temperature $k_B T_0/\hbar\omega_0$ as a function of the damping parameter α.

α	$\frac{k_B T_0}{\hbar\omega_0}$
0.00	0.155
0.02	0.152
0.05	0.148
0.10	0.141
0.25	0.122
0.50	0.096
1.00	0.065
2.00	0.037

At these high temperatures the trajectory $\bar{q}(t)$ in the inverted potential is a relatively small oscillation about q_0 (see Fig. 5). Similar conclusions hold in the dissipative case. The precise temperature above which Eq. (4.29) ceases to be valid is difficult to determine. Instead we shall determine the lowest temperature T_0 at which the action $S[\bar{q}]/\hbar$ is in a small range of the exponent of the classical escape process βV_0. The tunnel-rate formula should be valid for temperatures slightly lower than T_0.

To the extent that both quantum and classical escape processes are determined largely by the exponent of the appropriate escape-rate formula, T_0 corresponds to the temperature at which there is a crossover from the quantum-mechanical rate to the classical rate. The action obtained numerically enables us to determine T_0 for arbitrary values of the damping parameter α. We used the following method to determine T_0.

At a fixed value of α we selected an initial temperature that was low in the sense $\beta V_0 > S[\bar{q}]/\hbar$. The temperature was then increased until

$$\frac{\beta V_0 - S[\bar{q}]/\hbar}{S[\bar{q}]/\hbar} = 0.001 \ . \tag{5.16}$$

The temperature at which Eq. (5.16) holds serves as our definition of T_0. The choice of the numerical constant on the right-hand side of the above equation was determined by the accuracy to which $S[\bar{q}]$ was known.

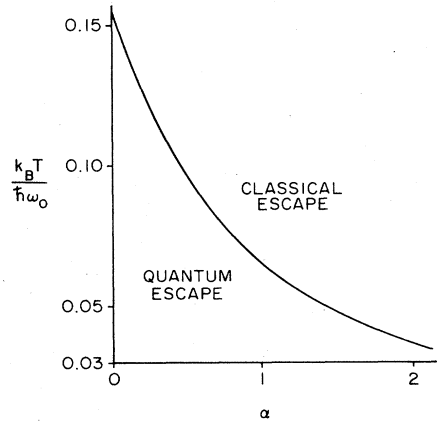

FIG. 8. Contour of crossover between quantum and classical escape in the (α, T) plane.

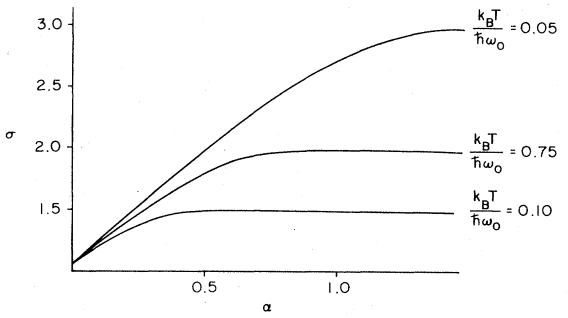

FIG. 9. Dimensionless action σ as a function of damping, α.

In Table I we present a range of values of the damping parameter α along with the corresponding values of the crossover temperature.

In the (α, T) plane of Fig. 8 we have drawn the contour where the crossover in behavior occurs; $T = T_0(\alpha)$. We have indicated the appropriate regions of the graph where the two different escape processes dominate. In Figs. 9 and 10 we show the behavior of the dimensionless action as a function of α at fixed T and as a function of T at fixed α. In Fig. 9 for sufficiently large α the action saturates to the classical exponent (i.e., $S[\bar{q}]/\hbar \to \beta V_0$). In Fig. 10 the action is seen to be relatively weakly dependent on temperature for low T. At higher temperatures it rapidly approaches the classical exponent.

Let us now consider the prefactor of the tunnel-escape-rate formula of Eq. (4.29),

$$A = \frac{1}{(2\pi\langle q^2\rangle)^{1/2}} \frac{||\dot{\bar{q}}||^2}{2m\,|\bar{q}(\tau/2)|} \times \left[\frac{\det''[-m\partial_t^2 + V''(\bar{q}(t)) + \hat{O}_t]}{\det(-m\partial_t^2 + m\omega_0^2 + \hat{O}_t} \right]^{-1/2} . \tag{5.17}$$

In terms of the dimensionless variables of Eqs. (5.3)—(5.6),

$$A = \omega_0 \frac{b}{2(2\pi\langle q^2\rangle)^{1/2}} \frac{||Z'||^2}{|Z''(\Omega/2)|} \times \left[\frac{\det''[-\partial_u^2 + 1 - 3Z(u) + \hat{O}_u]}{\det(-\partial_u^2 + 1 + \hat{O}_u)} \right]^{-1/2} , \tag{5.18}$$

where

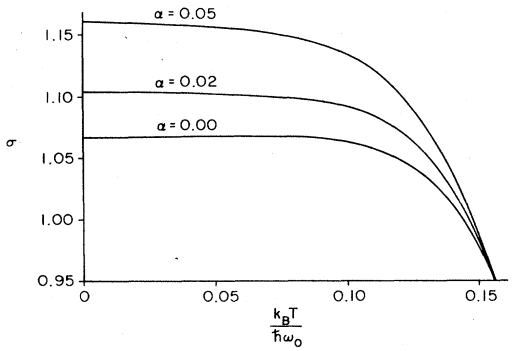

FIG. 10. Dimensionless action σ as a function of temperature.

$$||Z'||=\int_{-\Omega/2}^{\Omega/2} du\,[Z'(u)]^2 \tag{5.19}$$

and $\hat{O}_u$ is defined by

$$\hat{O}_u y(u)=\frac{2\alpha}{\pi}\int_{-\Omega/2}^{\Omega/2} dv \frac{y(u)-y(v)}{\left[\frac{\Omega}{\pi}\sin\left[\frac{\pi(u-v)}{\Omega}\right]\right]^2}\,. \tag{5.20}$$

All the factors in Eq. (5.18) multiplying the determinant ratio can be expressed in terms of known quantities and hence are also known, e.g.,

$$\frac{b}{2(2\pi\langle q^2\rangle)^{1/2}}=\left[\frac{m\omega_0 b^2}{2\hbar}\right]^{1/2}\times\left[\frac{\Omega}{4\pi}\frac{1}{\sum_n(\omega_n^2+2\alpha|\omega_n|+1)^{-1}}\right]^{1/2}, \tag{5.21}$$

$(\omega_n=2\pi n/\Omega)$,

$$||Z'||=\Omega\sum_n \omega_n^2 Z_n^2\,, \tag{5.22}$$

$$|Z''(\Omega/2)|=\sum_n(-1)^n\omega_n^2 Z_n^2\,. \tag{5.23}$$

These can be straightforwardly evaluated. All that remains to be determined is the determinant ratio.

Let us consider first the undamped ($\alpha=0$) determinant ratio. Defining

$$D\equiv\left[\frac{\det''(-m\partial_t^2+1-3Z(u)+\hat{O}_u)}{\det(-m\partial_t^2+1+\hat{O}_u)}\right]^{-1/2}, \tag{5.24}$$

we have for $T=0$ (i.e., $\Omega=\infty$)

$$D(\Omega=\infty,\alpha=0)=7.50\,, \tag{5.25}$$

and for $T=\hbar\omega_0/2\pi k_B$ (i.e., $\Omega=2\pi$)

$$D(\Omega=2\pi,\alpha=0)=\left[\frac{3\sinh(2\pi)}{4\pi}\right]^{1/2}\cong 7.99\,. \tag{5.26}$$

Equations (5.25) and (5.26) and explicit calculations for similar potentials make it more than plausible that D has, over the whole temperature range of interest, a variation of less than 7%.

For weak damping (say, $\alpha\lesssim 0.05$) the change in the results of Eqs. (5.25) and (5.26) is estimated to be as small as the error with which we can calculate this (12%), hence in this regime we make the approximation of replacing D by its zero-temperature, zero-damping limit, Eq. (5.25).

We can write the prefactor A [Eq. (5.18)] in terms of a dimensionless prefactor $F(\Omega,\alpha)$ defined by

$$A\equiv\omega_0\left[\frac{m\omega_0 b^2}{2\hbar}\right]^{1/2}F(\Omega,\alpha) \tag{5.27}$$

and in the above approximation we have

$$F(\Omega,\alpha)=\frac{15}{2}\left[\frac{\Omega}{4\pi}\frac{1}{\sum_n(\omega_n^2+2\alpha|\omega_n|+1)^{-1}}\right]^{1/2}\times\frac{||Z'||^2}{|Z''(\Omega/2)|}\,. \tag{5.28}$$

In Fig. 11 we show the behavior of $F(\Omega,\alpha)$ as a function of temperature at fixed α. The (unphysical) vanishing near the crossover temperature (as noted in the undamped case) is clearly manifested.

Let us now consider the prefactor for more general values of α. In this case the determinant ratio cannot be treated as a constant. The approach we adopt to evaluate the determinant ratio is similar to that used in Ref. 17 and is quite direct. We go to a matrix representation of the operators in Eq. (5.24), truncate the infinite matrices at finite order, and evaluate the determinants.

To obtain the matrix representation, we use the eigenfunctions of the undamped harmonic-oscillator operator (i.e., $-\partial_u^2+1$). These eigenfunctions satisfy the boundary conditions of vanishing at $\pm\Omega/2$ and are

$$\phi_n^A(u)=\left[\frac{2}{\Omega}\right]^{1/2}\sin(\omega_n u),\quad \omega_n=\frac{2\pi n}{\Omega}\,, \tag{5.29}$$

$$\phi_n^S(u)=\left[\frac{2}{\Omega}\right]^{1/2}\cos(\nu_n u),\quad \nu_n=\frac{(2n-1)\pi}{\Omega} \tag{5.30}$$

with $n=1,2,3,\ldots$.

After some calculation we find the following nonzero matrix elements:

$$\int_{-\Omega/2}^{\Omega/2} du\,\phi_m^A(u)[-\partial_u^2+1-3Z(u)+\hat{O}_u]\phi_n^A(u)$$
$$=(\omega_n^2+2\alpha|\omega_n|+1)\delta_{mn}+3(Z_{n+m}-Z_{n-m})\,, \tag{5.31}$$

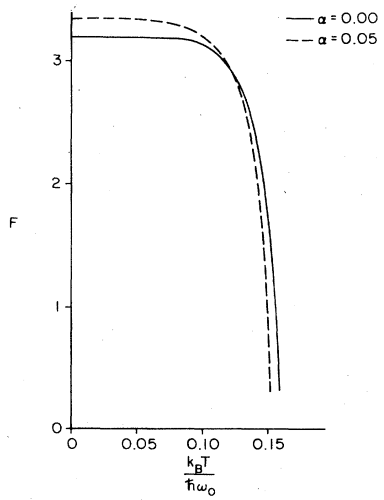

FIG. 11. Dimensionless prefactor F as a function of temperature.

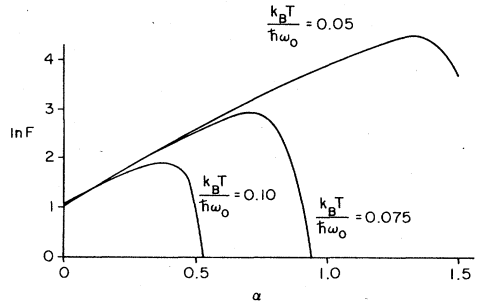

FIG. 12. Logarithm of the dimensionless prefactor F as a function of damping, α.

$$\int_{-\Omega/2}^{\Omega/2} du\, \phi_m^s(u)(-\partial_u^2+1-3Z(u)+\hat{O}_u)\phi_n^2(u)$$
$$=(\nu_n^2+1)\delta_{nm}-3(Z_{m+n-1}+Z_{m-n})$$
$$+\frac{32\alpha\nu_m\nu_n(-)^{m+n}}{\Omega^2}\sum_{P=1}^{\infty}\frac{\omega_p}{(\nu_m^2-\omega_p^2)(\nu_n^2-\omega_p^2)} \tag{5.32}$$

[The last term arises from expressing $\cos(\nu_n u)$ in terms of $\{\cos(\omega_p u)\}$.]

In principle, the above method can give the prefactor to arbitrary accuracy; it is only necessary to take sufficiently large matrices. We truncated the matrices at size 50×50 (and hence computed 100 eigenvalues). The error in the prefactor in the known region ($T\to 0, \alpha\to 0$) was found to be 12%. In Fig. 12 we plot the logarithm of the dimensionless prefactor $F(\Omega,\alpha)$ as a function of α at fixed T.

Since the qualitative behavior of the tunnel escape rate is dominated by the action of the exponent $S[\bar{q}]/\hbar$, we can qualitatively summarize the results of this section as follows.

(1) At fixed α the tunnel escape rate is an *increasing* function of T which approaches the classical escape rate.

(2) At fixed T the tunnel escape rate is a *decreasing* function of α. Increasing the damping (α) results in the tunnel escape rate decreasing to the classical escape rate.

VI. CONCLUSION

In this paper we have used an unorthodox method to calculate the rate of tunneling at finite temperatures out of a metastable potential well in the presence of dissipation. Our results for the exponent $S/\hbar$ in the expression equal to $A\exp(-S/\hbar)$ agree with those of other authors. With regard to the prefactor A, our results agree in the limit of zero dissipation with those obtained previously;[7] in the limit of zero temperature we have been (so far) unable to show analytically that they agree with the results of Ref. 11, but the numerical values obtained for the prefactor coincide within the accuracy of the calculation. The question of agreement or disagreement with the results[21,23] based on Eq. (1.9) for the case of finite dissipation and finite temperature remains an open one.

The astute reader will have noticed that, having criticized the use of Eq. (1.9) on the grounds that it may not adequately handle in a steady-state situation the effects of the finite relaxation time to the Boltzmann distribution, we have ourselves used a method of calculation which is vulnerable to the same criticism. This is because, in evaluating the density matrix under the barrier, we used the expression (4.5) corresponding to a thermal equilibrium distribution. However, we believe that the assumption embodied in Eq. (4.5) [or more precisely in its use to obtain Eq. (4.18)] is in some sense weaker than that necessary to obtain Eq. (1.9): the use of Eq. (1.9) requires, *prima facie* at least, that the thermal equilibrium Boltzmann distribution gives a correct account, to the accuracy required, of the imaginary *and real* parts of the free energy (or more precisely of the quantity which becomes the free energy in thermal equilibrium), our method, by contrast, requires only that it gives an adequate account of the (reduced) probability density near the far side of the barrier. Nevertheless, the physical assumptions (as distinct from the formal manipulations) are clearly closely related in the two methods, and we should remain open to the possibility that *neither* method will correctly give the prefactor for a genuinely "steady-state" situation. More generally, it could well be that (as may be the case in the Kramers problem) the correct expression to use for the prefactor in the tunneling rate will depend on the details of the way in which the system is prepared and allowed to come to equilibrium with its environment. We believe this question deserves further study.

We should emphasize, however, that this subtle technical point will affect only the detailed temperature and dissipation dependence of the prefactor, which is unlikely to play a major role in most real-life experimental situations; with regard to the dominant exponent in the tunneling rate, our formal expression agrees completely with those of other authors. Thus, our numerical evaluation of this exponent should be useful in the comparison of theory with experiment in this area, and should complement the analytical work of other authors.

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APPENDIX A: SEMICLASSICAL APPROXIMATION TO THE DENSITY MATRIX

In this appendix we briefly review the semiclassical approximation to the canonical density matrix. The unnormalized canonical density matrix for a particle at temperature $T=\hbar/k_B\tau$ with the Hamiltonian

$$H=\frac{p^2}{2m}+V(q) \tag{A1}$$

is[29]

$$\rho(q,q';\tau)=\sum_n \psi_n(q)\psi_n^*(q')e^{-E_n\tau/\hbar} \tag{A2}$$

$$=\int_{q',-\tau/2}^{q,\tau/2} d[q]e^{-S[q]/\hbar}, \tag{A3}$$

where

$$S[q]=\int_{-\tau/2}^{\tau/2} dr\left[\frac{m\dot{q}^2}{2}+V(q)\right] \tag{A4}$$

and the path integral of Eq. (A3) is over all trajectories starting at q' at time $-\tau/2$ and ending at q at time $+\tau/2$.

The semiclassical approximation is based on the fact that $S[q]$ has a minimum in function space about a trajectory $\bar{q}(t)$. This trajectory satisfies the extremum condition

$$\left.\frac{\delta S}{\delta q(t)}\right|_{\bar{q}}=0,\quad \bar{q}(-\tau/2)=q',\quad \bar{q}(\tau/2)=q\ . \tag{A5}$$

For the action of Eq. (A4) the extremum condition is

$$m\ddot{\bar{q}}(t)-V'(\bar{q}(t))=0\ . \tag{A6}$$

Note the minus sign in front of the potential. This equation evidently corresponds to the classical motion of a particle which moves in the potential $-V(q)$, the *inverted* potential.

In Eq. (A3) we write

$$q(t)=\bar{q}(t)+y(t),\quad y(\pm\tau/2)=0\ , \tag{A7}$$

hence

$$S[q]=S[\bar{q}+y]=S[\bar{q}]+\frac{1}{2!}\int_{-\tau/2}^{\tau/2}ds\int_{-\tau/2}^{\tau/2}dt\left.\frac{\delta^2 S}{\delta q(s)\delta q(t)}\right|_{\bar{q}} y(s)y(t)+\cdots\ . \tag{A8}$$

The semiclassical approximation is made by simply truncating the functional Taylor series in $y(t)$ at quadratic order. The semiclassical approximation to $\rho(q,q';\tau)$ is then

$$\rho(q,q';\tau)=e^{-S[\bar{q}]/\hbar}\int_{0,-\tau/2}^{0,\tau/2} d[y]\exp\left[-\frac{1}{2\hbar}\int_{-\tau/2}^{\tau/2}dt\left.\frac{\delta^2 S}{\delta q(t_1)\delta q(t_2)}\right|_{\bar{q}} y(t_1)y(t_2)\right]\ . \tag{A9}$$

The integral in Eq. (A9) is a Gaussian which can be evaluated by expressing $y(t)$ in terms of a complete set of orthonormal functions $\{\phi_n\}$ satisfying $\phi_n(\pm\tau/2)=0$,

$$y(t)=\sum_n c_n\phi_n(t)\ , \tag{A10}$$

and furthermore the $\{\phi_n\}$ are chosen to be eigenfunctions of the Hermitian operator

$$\left.\frac{\delta^2 S}{\delta q(t_1)\delta q(t_2)}\right|_{\bar{q}}\ .$$

That is, each eigenfunction obeys

$$\int_{-\tau/2}^{\tau/2}dt_2\left.\frac{\delta^2 S}{\delta q(t_1)\delta q(t_2)}\right|_{\bar{q}}\phi_n(t_2)=\lambda_n\phi_n(t_1)\ ,$$

$$\phi_n(\pm\tau/2)=0,\quad \int_{-\tau/2}^{\tau/2}dr\,\phi_n(t)\phi_m(t)=\delta_{nm}\ . \tag{A11}$$

Using equations (A10) and (A11), we can write Eq. (A9) as

$$\rho(q,q';\tau)=e^{-S[\bar{q}]/\hbar}N\int\prod_n\frac{dc_n}{\sqrt{2\pi\hbar}}\exp\left[-\frac{1}{2\hbar}\sum\lambda_n c_n^2\right], \tag{A12}$$

where

$$d[y]=N\prod_n\frac{dc_n}{\sqrt{2\pi\hbar}}\ . \tag{A13}$$

Evaluating the integrals in Eq. (A12), we obtain

$$\rho(q,q';\tau)=N\left[\prod_n\lambda_n^{-1/2}\right]e^{-S[\bar{q}]/\hbar}\ . \tag{A14}$$

For the action of Eq. (A4) the eigenvalue equation (A11) can be written as

$$[-m\partial_t^2+V''(\bar{q}(t))]\phi_n(t)=\lambda_n\phi_n(t)\ ,$$

$$\partial_t\equiv\frac{\partial}{\partial t}\ . \tag{A15}$$

In view of this we can write Eq. (14) as

$$\rho(q,q';\tau)=N\det{}^{-1/2}[-m\partial_t^2+V''(\bar{q}(t))]e^{-S[\bar{q}]/\hbar}\ . \tag{A16}$$

Implicitly we have assumed that a unique trajectory $\bar{q}(t)$ satisfies Eq. (A5). In the case of several distinct extrema (minima) we add their individual contributions to obtain

$$\rho(q,q';\tau)=\sum_j N\det{}^{-1/2}[-m\partial_t^2+V''(\bar{q}(t))]e^{-S[\bar{q}]/\hbar}\ . \tag{A17}$$

This is the semiclassical approximation to the canonical density matrix. This is expected to be valid whenever the average quadratic fluctuations about an extremal trajectory are small compared with characteristic length scales of the potential $V(q)$.

APPENDIX B: BEHAVIOR OF $E'_{\rm cl}(\tau)$

In this appendix we investigate the derivative of the energy $\partial E_{\rm cl}/\partial\tau$. $E_{\rm cl}$ is the solution of

$$T_{\rm cl}(E_{\rm cl})=\tau\ , \tag{B1}$$

where

$$T_{\rm cl}(E)\equiv\sqrt{2m}\int_{q_1}^{q}\frac{dq'}{[V(q')-E]^{1/2}} \tag{B2}$$

and q_1 is defined by $V(q_1)=E$. $T_{\rm cl}(E_{\rm cl})$ is the period of the motion given in Fig. 5.

It will be convenient to evaluate not $E'_{\rm cl}(\tau)$, but rather its reciprocal

$$T'_{\rm cl}(E_{\rm cl})=\left.\frac{\partial T_{\rm cl}(E)}{\partial E}\right|_{E_{\rm cl}}.$$

We rewrite Eq. (B2) in a form that makes it straightforward to differentiate $T_{\rm cl}(E)$ with respect to E. We use the identity

$$[V(q)-E]^{-1/2}\equiv\frac{2}{V'(q)}\frac{\partial}{\partial q}[V(q)-E]^{1/2} \tag{B3}$$

to write

$$T_{\rm cl}(E)=2\sqrt{2m}\int_{q_1}^{q}dq'\frac{1}{V'(q')}\frac{\partial}{\partial q'}[V(q')-E]^{1/2} \tag{B4}$$

$$\equiv 2\sqrt{2m}\int_{q_1}^{q}dq'\frac{1}{V'(q')}\frac{\partial}{\partial q'}\times\{[V(q')-E]^{1/2}-[V(q_0)-E]^{1/2}\}\ , \tag{B5}$$

where q_0 corresponds to the maximum of the barrier [$V'(q_0)=0$, see Fig. 5]. Integrating (B5) by parts yields

$$T_{\rm cl}(E)=2\sqrt{2m}\left[\frac{[V(q)-E]^{1/2}-[V(q_0)-E]^{1/2}}{V'(q)}+\frac{[V(q_0)-E]^{1/2}}{V'(q_1)}\right]$$
$$+2\sqrt{2m}\int_{q_1}^{q}dq'\frac{V''(q')}{[V'(q')]^2}\{[V(q')-E]^{1/2}-[V(q_0)-E]^{1/2}\}\ . \tag{B6}$$

Equation (B6) is in a form that can be differentiated with respect to E. Doing so, and defining

$$\dot{\bar{q}}(q)\equiv\left[\frac{2}{m}[V(q)-E]\right]^{1/2}, \tag{B7}$$

we obtain for $q>q_0$

$$|T'_{\rm cl}(E_{\rm cl})|=\chi(q,\tau)\frac{\dot{\bar{q}}(q)-\Delta}{\dot{\bar{q}}(q)}\ , \tag{B8}$$

where

$$\chi(q,\tau)\equiv 2\int_{q_1}^{q}dq'\frac{V''(q')}{[V'(q')]^2}\left[\frac{1}{\dot{\bar{q}}(q')}-\frac{1}{\dot{\bar{q}}(q_0)}\right]+\frac{2}{\dot{\bar{q}}(q_0)}\left[\frac{1}{V'(q_1)}-\frac{1}{V'(q)}\right] \tag{B9}$$

and

$$\Delta\equiv\frac{2}{\chi(q,\tau)\,|V'(q)|}\ . \tag{B10}$$

We can repeat the above calculation for the periodic orbit (i.e., the trajectory of Fig. 5 that starts and ends at $q_p(\tau)$ with zero velocity and takes a time τ to achieve this). The energy of this orbit is $-E_p(\tau)$ and is the solution of

$$T_p(E_p)=\tau\ , \tag{B11}$$

where

$$T_p(E)\equiv\sqrt{2m}\int_{q_1}^{q_p}\frac{dq'}{[V(q')-E]^{1/2}} \tag{B12}$$

and $q_p(\tau)$ is defined by $V(q_p)=E_p(\tau)$.

After some calculation we find

$$|T'_p(E_p)|=\chi(q_p(\tau),\tau) \tag{B13}$$

with χ again given by Eq. (B9). For q close to $q_p(\tau)$, Eqs. (B8), (B9), (B10), and (B13) give

$$|T'_{\rm cl}(E_{\rm cl})|\cong\left[\frac{\dot{\bar{q}}(q)-\Delta}{\dot{\bar{q}}(q)}\right]|T'_p(E_p)| \tag{B14}$$

with

$$\Delta\cong\frac{2}{|T'_p(E_p)|\,|V'(q_p)|}\ . \tag{B15}$$

APPENDIX C: DIAGONAL ELEMENTS OF THE REDUCED HARMONIC-OSCILLATOR DENSITY MATRIX

In this appendix we obtain the diagonal elements of the reduced density matrix for a harmonic oscillator subject to dissipation. The required quantity is

$$\rho_0(q,q;\tau)=\int_{q,-\tau/2}^{q,\tau/2}d[q]e^{-S[q]/\hbar} \tag{C1}$$

with

$$S[q]=\int_{-\tau/2}^{\tau/2}dt\left[\frac{m\dot{q}^2}{2}+\frac{m\omega_0^2q^2}{2}\right]+\frac{\eta\pi}{4\tau^2}\int_{-\tau/2}^{\tau/2}ds\int_{-\tau/2}^{\tau/2}dt\left[\frac{q(t)-q(s)}{\sin\left[\frac{\pi(t-s)}{\tau}\right]}\right]^2. \tag{C2}$$

The semiclassical approximation to $\rho_0(q,q,\tau)$ is exact since $S[q]$ is quadratic in $q(t)$. From Eq. (4.14) we have

$$\rho_0(q,q';\tau)=N\det{}^{-1/2}[-m\partial_t^2+m\omega_0^2+\hat{O}_t]e^{-S[\bar{q}]/\hbar}\ . \tag{C3}$$

Decomposing $\bar{q}(t)$ into a Fourier sum as in Ref. 11,

$$\bar{q}(t)=\sum_{n=-\infty}^{\infty} q_n e^{i\nu_n t},\quad \nu_n=\frac{2\pi n}{\tau} \tag{C4}$$

yields for the action

$$\frac{S[\bar{q}]}{\hbar}=\frac{m\tau}{2\hbar}\sum(\nu_n^2+2\gamma\,|\,\nu_n\,|\,+\omega_0^2)q_n^2,\quad \gamma\equiv\frac{\eta}{2m}\ . \tag{C5}$$

The $\{q_n\}$ are determined by using the fact that the action is stationary to first-order variations of the $\{q_n\}$ subject to the constraint

$$\bar{q}(\pm\tau/2)=q=\sum(-1)^n q_n\ . \tag{C6}$$

The variation is

$$\frac{\partial}{\partial q_n}\sum_n[(\nu_n^2+2\gamma\,|\,\nu_n\,|\,+\omega_0^2)q_n^2-2\lambda(-1)^n q_n]=0\ , \tag{C7}$$

where λ is a Lagrange multiplier.

Equations (C6) and (C7) yield

$$q_n=q(-1)^n\frac{(\nu_n^2+2\gamma\,|\,\nu_n\,|\,+\omega_0^2)^{-1}}{\sum_n(\nu_n^2+2\gamma\,|\,\nu_n\,|\,+\omega_0^2)^{-1}}\ . \tag{C8}$$

Hence the action is

$$\frac{S[\bar{q}]}{\hbar}=\frac{mq^2\tau}{2\hbar}\frac{1}{\sum_n(\nu_n^2+2\gamma\,|\,\nu_n\,|\,+\omega_0^2)^{-1}}\ . \tag{C9}$$

Introducing

$$\langle q^2\rangle\equiv\frac{\hbar}{m\tau}\sum_n(\nu_n^2+2\gamma\,|\,\nu_n\,|\,+\omega_0^2)^{-1} \tag{C10}$$

$$=\frac{\hbar}{m\pi}\int_0^\infty d\omega\coth\frac{\omega\tau}{2}\frac{2\gamma\omega}{(\omega_0^2-\omega^2)^2+(2\gamma\omega)^2} \tag{C11}$$

enables the action to be written as

$$\frac{S[\bar{q}]}{\hbar}=\frac{q^2}{2\langle q^2\rangle}\ . \tag{C12}$$

Hence Eq. (C3) is

$$\rho_0(q,q;\tau)=N\det{}^{-1/2}(-m\partial_t^2+m\omega_0^2+\hat{O}_t)e^{-q^2/2\langle q^2\rangle}\ , \tag{C13}$$

the required result.

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