

Incoherent tunneling in a double well

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We give a detailed presentation of a method for calculating the rate of incoherent tunneling between the minima of damped systems, described by a double-well potential. The method does not require that the dynamics of the system be truncated onto a two-state model. This has the advantage that all the quantities that enter into our final expression for the tunneling rate, especially the prefactor, are defined in terms of the parameters describing the potential well and the dissipation strength. We present a model potential for which all the necessary steps can be performed exactly, within the semiclassical limit. We obtain an exact expression for the decay rate that can be compared with estimates used in the context of the truncation schemes. The exponential part of the tunneling rate agrees quite well with the truncation-scheme approximations. However, there have been no corresponding estimates of the behavior of the prefactor. We find an exact expression for this prefactor, which shows only a very weak dependence on the strength of the dissipation mechanism. This is in strong contrast to the dependence of the prefactor for the tunneling decay of a metastable state into a continuum.

I. INTRODUCTION

Many physical and chemical systems can be described by a generalized coordinate and an effective potential which has almost degenerate minima. Such systems are frequently coupled to a heat bath, allowing the system to enter a state of thermal equilibrium. There has been a great amount of interest in the dynamics of such systems due to the diversity of physical realizations as well as to some recent advances in the theory.¹⁻¹³ Most of the previous studies of the dynamics of dissipative systems, described by double-well potentials, have relied on simplifying assumptions. One assumption that is most often utilized is that, at sufficiently low temperatures, the dynamics only involves the ground states of the potential minima. Thus, when the system is decoupled from the heat bath, the dynamics can be described in a two-dimensional Hilbert space.

Several authors have investigated the circumstances under which the dissipative dynamics of a double well may be reduced to that of a two-state problem. Reduction schemes have been frequently used to treat tunneling centers in solids.¹ The case in which the coupling to the heat bath is of ohmic form has been studied by several groups,²⁻⁶ using the two-state description. Simultaneously, Weiss *et al.*^{7,8} have presented a method of treatment for the double-well system, which does not use the two-state model as an intermediate step. The calculations^{7,8}

were performed directly on the model system and not on the approximate two-state model.

In this paper we present our method^{7,8} in greater detail. We shall also apply this method to the calculation of the incoherent tunneling rate, for a model potential. An explicit analytic expression for the tunneling rate is obtained and is evaluated, without invoking any further approximations, beyond the semiclassical approximation.

The paper is organized as follows. In Sec. II we shall present a detailed description of our method of calculating the tunneling rate for a biased double-well potential. The method is based on a similar approach to decay problems, originally due to Langer. In Sec. III we present the model potential which we shall study in greater detail. We shall evaluate the family of trajectories which dominate the dynamics of the decay process in Sec. III A. In Sec. III B we shall calculate the exponential part of the decay rate due to these trajectories. In Sec. IV we shall calculate the prefactor of the tunneling rate, by relating it to the T matrix of scattering theory. In Sec. IV A we shall find this T matrix exactly and in Sec. IV B we shall evaluate the prefactor. In Sec. V, we examine the various limits of the tunneling rate and compare them to estimates made in the context of the two-state truncation schemes. The exponential parts of the tunneling rate are in good agreement with the estimates. The truncation schemes are, however, unable to predict the value of the prefactor or its dependence on the strength of the dissipation. We discuss this in detail and summarize our results.

II. THE INSTANTON SUM FOR A BIASED DOUBLE WELL

We consider a system which has its relevant dynamics described by a macroscopic variable q and may be conceptualized as a particle of mass M moving in a potential field $V(q)$. We assume that the potential $V(q)$ is a slightly asymmetric double-well potential, in which the minima are located at $q = \pm q_0/2$. The minima are separated by a potential barrier of height V_0 , as shown in Fig. 1. The frequency of the small amplitude oscillations of q , at the potential minima of the undamped system, is given by $\omega_0 = [V''(\pm q_0/2)/M]^{1/2}$. The bias energy $\hbar\sigma$, defined by $\hbar\sigma = V(-q_0/2) - V(q_0/2)$ is assumed to be such that $\sigma \ll \omega_0$.

In the absence of dissipation, the two lowest eigenstates of the system are separated by an energy $\hbar\Delta_b = \hbar(\sigma^2 + \Delta_0^2)^{1/2}$, where $\hbar\Delta_0$ is the bare tunnel splitting of the unbiased double well. This may be calculated using the standard WKB techniques, yielding

$$\Delta_0 = \omega_0 B (q_0/a_0) \exp(-CV_0/\hbar\omega_0),$$

when $V_0 \gg \hbar\omega_0$. In this expression $a_0 = (\hbar/2M\omega_0)^{1/2}$ is the root-mean-square displacement of the zero-point fluctuations in the well; and B, C are constants, of order unity, which depend on the shape of the barrier.

In what follows, we shall restrict our investigations to the limit

$$V_0 \gg \hbar\omega_0 \gg |\hbar\sigma|, \quad \hbar\omega_0 \gg k_B T. \quad (2.1)$$

Under these conditions, we expect that the system may be reasonably described by a biased two state model since the excited states of both the wells may be neglected.

Let $P_L(t)$ [$P_R(t)$] denote the probability that the particle, initially in the left-hand well at time $t=0$, is found in the left-hand (right-hand) well at a later time t . The dynamics of such a system is conveniently characterized by the relative occupation probability,

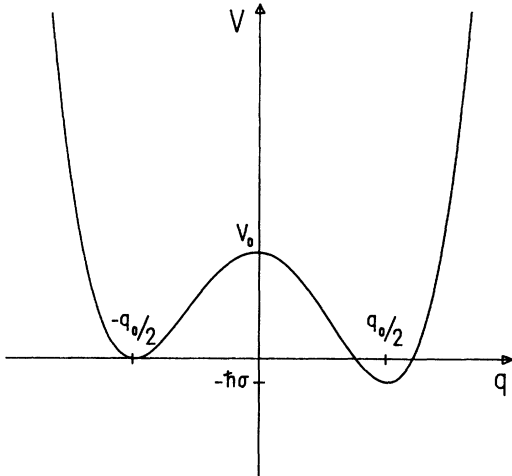


FIG. 1. An asymmetric double-well potential $V(q)$. The potential minima are located at $\pm q_0/2$, and have a slight asymmetry in their depth of $-\hbar\sigma$. The height of the potential barrier is V_0 .

$$P(t) = P_L(t) - P_R(t). \quad (2.2)$$

In the absence of coupling to the heat bath, $P(t)$ exhibits an oscillatory behavior with increasing time

$$P(t) = \left[\frac{\sigma}{\Delta_b} \right]^2 + \left[\frac{\Delta_0}{\Delta_b} \right]^2 \cos(\Delta_b t). \quad (2.3)$$

The dynamics of the system is strongly affected by the dissipative mechanism caused by coupling to the heat baths dynamical degrees of freedom. Such damping phenomena are always expected to be present whenever the tunneling system is part of a macroscopic body. We shall consider linear couplings to the heat bath, that are associated with the phenomenological classical equation of motion

$$\ddot{q}(t) + \int_0^t ds \gamma(t-s) \dot{q}(s) + M^{-1} \frac{\partial V}{\partial q} = 0, \quad (2.4)$$

in which $\gamma(t)$ is a phenomenological damping kernel. For Ohmic damping, the kernel $\gamma(t)$ is proportional to a Dirac δ function $\delta(t)$.

The influence of damping on the coherent oscillations of equation (2.3) have been studied by various authors.^{2,6,8-13} It is found that these oscillations only survive at short times, and with appreciable amplitude for the small corner of space characterized by the conditions

$$\alpha_c < \frac{1}{2}, \quad \alpha_c k_B T \ll \hbar\Delta_0, \quad \sigma < \Delta_0, \quad (2.5)$$

where α_c is a dimensionless dissipation constant

$$\alpha_c = \frac{M\gamma q_0^2}{2\pi\hbar}. \quad (2.6)$$

This regime is that of quantum coherence, which was recently investigated.^{2,6,9-11,13} In this paper, we shall not address this regime, but instead shall investigate the regime under which the damping changes the behavior of $P(t)$ to that of purely incoherent exponential relaxation^{5,8,9} described by

$$P(t) = P_\infty + (1 - P_\infty) \exp(-\Gamma t) \quad (2.7)$$

where $P_\infty = -\tanh(\hbar\beta\sigma)/2$ is the thermal equilibrium value of $P(t)$. In this expression, $\Gamma = \Gamma_+ + \Gamma_-$ is the total relaxation rate which is given in terms of the sum of forward, Γ_+ , and the backward, Γ_- , tunneling rates.⁸ The term $\beta = 1/k_B T$. In the regime where (2.7) applies, the time evolution of the system can be described in terms of the rates for transitions between the wells, so that the probabilities $P_L(t)$ and $P_R(t)$ may be described by a classical stochastic process. That means the nature of the process is similar to the processes which can be described by a Pauli master equation,¹⁴ although there are important differences due to the fact that the transitions are not between the energy eigenstates and that the transition rates cannot be calculated by treating the coupling as a perturbation.¹⁵

In general, the dynamics of a dissipative double well must be described in real time, e.g., by using functional-integral methods of the Feynman-Vernon type.¹⁶ However, in the incoherent regime it is sufficient to calculate the

transition rates microscopically and then determine the dynamics using a master equation.¹⁷ The transition rates can be determined by analytically continuing the free energy from a stable to a metastable state. This method was developed by Langer¹⁸ in connection with nucleation theory and later applied to problems involving quantum decay, by Callan and Coleman.¹⁹ Although a general justification of this method does not exist, it has been found for the case of incoherent tunneling that the method produces results that are identical to those obtained by means of more complicated procedures.²⁰

In the remainder of this section, we present a functional integral method to calculate the imaginary part of the free energy of the metastable state of the double-well system. The rate of tunneling transitions out of the metastable state is assumed to be proportional to the imaginary part of this analytically continued free energy.²¹ The method involves a summation over the so-called "instanton" trajectories. The instanton summation was discussed in detail by Zinn-Justin²² for the undamped systems. Instantons were first used by Weiss *et al.*⁷ in the case of damping, to treat quantum decay into a continuum. Later, Weiss and Grabert have utilized this method to investigate the damped quantum dynamics of a particle in a double well^{8,9} and a periodic potential.⁸ The presentation below gives a more detailed account of the approach used in Ref. 8.

The free energy F is related to the partition function Z through the relation

$$F = -\beta \ln Z,$$

and this latter quantity may be written in terms of an Euclidean functional integral²³

$$Z = \int \mathcal{D}[q(\tau)] \exp\{-S[q(\tau)]/\hbar\}, \quad (2.8)$$

where the paths to be summed have to be periodic, i.e., $q(0)=q(\theta)$, where $\theta=\hbar\beta$. These paths are weighted by the Euclidean action

$$S[q(\tau)] = S_0[q(\tau)] + S_d[q(\tau)], \quad (2.9)$$

where S_0 is the action in the absence of dissipation and S_d is a nonlocal action describing the dissipation. The action S_0 is given by the expression

$$S_0[q(\tau)] = \int_{-\theta/2}^{\theta/2} d\tau \left[\frac{M}{2} \dot{q}^2 + V(q) \right]. \quad (2.10)$$

The nonlocal dissipative part of the action is given by²³⁻²⁶

$$S_d[q(\tau)] = \frac{1}{2} \int_{-\theta/2}^{\theta/2} d\tau \int_{-\theta/2}^{\theta/2} d\tau' k(\tau-\tau') q(\tau) q(\tau'). \quad (2.11)$$

Caldeira and Leggett²⁴ have determined the dissipative kernel $k(\tau)$ from a microscopic model by integrating out the normal modes of the heat bath. For a system with a linear dissipative mechanism, the form of $S_d[q(\tau)]$ can also be inferred from a purely phenomenological basis, as shown by Grabert and Weiss.²⁵ In either case, one finds that $k(\tau)$ is related to the phenomenological damping kernel $\gamma(t)$ by

$$k(\tau) = \frac{M}{\theta} \sum_{n=-\infty}^{+\infty} |\omega_n| \tilde{\gamma}(|\omega_n|) \exp(i\omega_n \tau), \quad (2.12)$$

where $\omega_n = 2\pi n/\theta$ are the Matsubara frequencies and $\tilde{\gamma}(z)$,

$$\tilde{\gamma}(z) = \int_0^\infty dt \exp(-zt) \gamma(t), \quad (2.13)$$

is the Laplace transform of the phenomenological damping kernel. In the microscopic model $\tilde{\gamma}(z)$ is related to the spectral density $J(\omega)$ of the coupling to the heat bath^{24,25} through

$$\tilde{\gamma}(z) = \frac{2}{\pi M} \int_0^\infty d\omega \frac{z}{\omega^2 + z^2} \frac{J(\omega)}{\omega}. \quad (2.14)$$

In the case of Ohmic dissipation, the damping coefficient $\tilde{\gamma}(z)$ is frequency independent at low frequencies, i.e., $\tilde{\gamma}(z) = \gamma$. This behavior is obtained when the spectral density $J(\omega) = M\gamma\omega$ for small ω .

The functional integral expression for the partition function (2.8) is to be evaluated with the weakly biased double well potential sketched in Fig. 1. The main contributions to the path integral come from the periodic paths for which the action is extremal. Clearly, the largest contribution arises from the paths that remain at the minima of the potential. However, the interesting physics of the decay process is associated with the paths that traverse the classically forbidden region between the wells.

The paths which extremalize the action (2.9) satisfy the Euler-Lagrange equation

$$-M\ddot{q}(\tau) + \frac{\partial V}{\partial q} + \int_{-\theta/2}^{\theta/2} d\tau' k(\tau-\tau') q(\tau') = 0. \quad (2.15)$$

The action evaluated along the extremal path may be transformed to read

$$S_{\text{ex}} = \int_{-\theta/2}^{\theta/2} d\tau \left[V(q) - \frac{1}{2} q \frac{\partial V}{\partial q} \right] \quad (2.16)$$

in which we have utilized (2.15).

The partition function (2.8) can be written in terms of the contributions from these extremal paths and the small fluctuations around them. In the absence of dissipation, it is the path which traverses the classically forbidden region just once that leads to the tunnel splitting of the energy levels. For a system with Ohmic dissipation the situation is complicated by an infrared divergence that appears in the theoretical description. We shall briefly contrast these two situations, and display the origin of the divergence.

First for simplicity, we consider the case in which $\sigma=0$ and $T=0$, so that $\theta \rightarrow \infty$ and the potential is symmetric. The instanton trajectory $q_I(\tau)$ which extremalizes the action, starts at $\tau = -\infty$ at $q_I(-\infty) = -q_0/2$ and ends up at $q_I(\infty) = +q_0/2$ when $\tau \rightarrow +\infty$. The instanton is centered at $\tau=0$, so that $q_I(-\tau) = -q_I(\tau)$. We choose a time scale τ_0 sufficiently large such that for $|\tau| > \tau_0$, the trajectory $q_I(\tau)$ is in the region where the potential is approximately harmonic. Then the action can be rewritten as the sum

$$S_I = S_I^0 + S_I^{\text{as}}$$

in which S_I^0 and S_I^{as} are the contributions from times

$|\tau| < \tau_0$ and $|\tau| > \tau_0$, respectively. The action arising from the asymptotic, large τ , part of the trajectory can be written as

$$S_I^{\text{as}} = \frac{1}{2} M \omega_0^2 q_0 \int_{\tau_0}^{\infty} d\tau \left[\frac{1}{2} q_0 - q_I(\tau) \right]. \quad (2.17)$$

For the undamped system, the instanton approaches $q_0/2$ exponentially fast as $\tau \rightarrow \infty$. Hence, S_I^{as} is a well-defined finite quantity in the absence of dissipation. This is in sharp contrast to the case where ohmic dissipation is present. For Ohmic dissipation one finds that the kernel $k(\tau)$ in the nonlocal part of the action has an asymptotic algebraic decay: $k(\tau) \sim \tau^{-2}$. From the equation of motion (2.15), one finds that the instanton approaches the bottom of the well algebraically slowly,

$$\frac{1}{2} q_0 - q_I(\tau) \sim \tau^{-1}$$

as $\tau \rightarrow \infty$. Hence, the intrainstanton interaction due to the dissipative coupling gives rise to a power-law decay of the instantons amplitude, at large times. As a consequence, S_I^{as} diverges in the ohmic case. This is the infrared divergence arising from the coupling to the low-frequency modes of the heat bath. When the spectral density $J(\omega)$ vanishes faster than ω as $\omega \rightarrow 0$, the instanton amplitude decays faster than τ^{-1} so that S_I^{as} remains finite. Thus for non-Ohmic damping the functional integral expression for the partition function may be treated in basically the same way as for the undamped case. In particular, the instanton action can be used to define a tunnel splitting Δ , in much the same way as it is defined for the undamped double well.²² Naturally, due to the dissipative intrainstanton interaction, Δ will differ from Δ_0 by a factor of the Debye-Waller type. The main conclusion is that non-Ohmic damping does not qualitatively change the low-temperature dynamics of the double well. The quantity $P(t)$ will still show an oscillatory behavior, although the heat bath renormalizes the oscillation frequency and leads to a decay of the amplitude.

For the case of the ohmic damping the corresponding functional integral expression for the partition function must be evaluated with more care. Fortunately, the path integral (2.8) is to be evaluated by summing over periodic paths, so that each instanton is followed by an anti-instanton. Such a configuration will, henceforth, be referred to as an extended bounce.⁷ The extended bounce trajectory has an internal degree of freedom, the bounce length τ_1 which is the relative separation of the instanton—anti-instanton pair forming the bounce (cf. Fig. 2). As we shall see, the action S_B associated with an extended bounce, is finite. To show this, consider the $T=0$ bounce starting at $\tau \rightarrow -\infty$ at $q_B(-\infty) = -q_0/2$, penetrating through the potential barrier and returning to the initial point at time $\tau \rightarrow +\infty$. The trajectory passes the position of the maximum barrier height at the times $\tau = \pm \tau_1/2$ [cf. Fig. 2]. If we again denote the time interval of a traversal of the classically forbidden region by τ_0 , the bounce trajectory is in the harmonic region of the potential for all τ such that $|\tau| > \frac{1}{2}\tau_1 + \tau_0$ or $|\tau| < \frac{1}{2}\tau_1 - \tau_0$. (The typical bounce length τ_1 will turn out to be large compared to the width of the instanton which is basically τ_0 .) For finite τ_1 , the action may only

diverge due to the asymptotic parts of the trajectory, i.e., $|\tau| > \frac{1}{2}\tau_1 + \tau_0$. The asymptotic part of the trajectory contributes a term

$$S_B^{\text{as}} = \frac{1}{2} M \omega_0^2 q_0 \int_{\tau_1/2 + \tau_0}^{\infty} d\tau \left[\frac{1}{2} q_0 + q_B(\tau) \right] \quad (2.18)$$

to the action. Just as in the case of the single instanton, which we discussed previously, the asymptotic decay of the trajectory is strongly influenced by the self-interaction, caused by the dissipation. However, we now have an instanton—anti-instanton pair which traverse the potential barrier in opposite directions. This results in a partial cancellation of their influence upon the asymptotic parts of the trajectory. As we shall see in the next section, in the Ohmic case, the amplitude of the bounce decays as $q_B(\tau) + \frac{1}{2}q_0 \sim \tau^{-2}$ [Eq. (3.15); see also p. 2195 in Ref. 26] so that the asymptotic part of the bounce action (2.18) is convergent. (Note that for a single instanton τ^{-2} would be replaced by τ^{-1} .) Thus, the infrared problem associated with the instanton action can be avoided by grouping the $2n$ instanton—anti-instantons into n extended bounces.

Next, we shall evaluate the partition function for the metastable state which is mainly confined to the well located at $q = -q_0/2$, i.e., on the left. We denote this quantity by Z_L . The quantity Z_L is given by the functional integral (2.8) evaluated as the sum of periodic trajectories which remain mostly near $q = -q_0/2$, except for rare excursions into the well at $q = +q_0/2$. Besides the trajectories which are confined within the well at $q = -q_0/2$ at all times, there are tunneling trajectories that traverse the potential barrier $2n$ times, where n is a positive integer. To determine the contribution of these tunneling trajectories to Z_L , we have to evaluate the action due to all the multi-instanton trajectories and their neighboring paths.

We shall assume that the instanton—anti-instanton of a configuration comprised of n neighboring instanton—anti-instanton pairs are located at the times $\tau = s_j$, where $j = 1, 2, \dots, 2n$. Each instanton starting from $q = -q_0/2$ is combined with the subsequently following anti-instanton which returns to $q = -q_0/2$, to form an extended bounce. Once this grouping into bounces has been per-

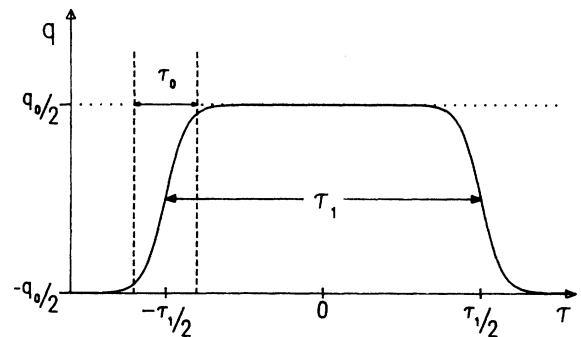


FIG. 2. A bounce trajectory. The instanton and anti-instanton parts of the trajectory have typical widths τ_0 and are located at $-\tau_1/2$ and $+\tau_1/2$, respectively.

formed, it is convenient to separate the action of an n bounce configuration into intrabounce actions and inter-bounce interactions. To do this it is convenient to rewrite the dissipative part of the action as

$$S_d[q(\tau)] = -\frac{1}{2} \int_{-\theta/2}^{\theta/2} d\tau \int_{-\theta/2}^{\theta/2} d\tau' l(\tau-\tau') \dot{q}(\tau) \dot{q}(\tau') \quad (2.19)$$

by performing two partial integrations. The kernel $l(\tau)$ is related to $k(\tau)$ through

$$\frac{\partial^2 l}{\partial \tau^2}(\tau) = k(\tau).$$

For strictly Ohmic dissipation, i.e., $J(\omega) = M\gamma\omega$, we find that

$$l(\tau) = \frac{M\gamma}{\pi} \ln \left| \frac{\theta\omega_d}{\pi} \sin \left[\frac{\pi\tau}{\theta} \right] \right|, \quad (2.20)$$

where ω_d is an arbitrary frequency arising from the partial integration. Since the paths $q(\tau)$ are periodic, $S_d[q(\tau)]$ is independent of the choice of ω_d . In the limit of low temperatures, where θ is very large compared with the instanton width τ_0 , the interaction between two instantons mediated by the dissipation (2.19) can be calculated in the sudden flip approximation, in which the velocity of the $2n$ instanton configuration is approximated by a series of δ functions. Using the periodicity of the trajectory, we may always start the sequence of flips with an instanton. Thus we have the approximation

$$\dot{q}_{2n}(\tau) = \sum_{j=1}^n (-1)^{j+1} q_0 \delta(\tau - s_j). \quad (2.21)$$

With the aid of this approximation, we may rewrite (2.19) as

$$S_d[q_{2n}(\tau)] = 2n S_I^{\text{self}} + \sum_{\substack{j,k=1 \\ (j < k)}}^{2n} (-1)^{j+k+1} P(s_k - s_j) \hbar, \quad (2.22)$$

in which S_I^{self} is the self-interaction of an instanton due to the nonlocal dissipation term. This term, S_I^{self} , cannot be treated in the sudden flip approximation. The section sum gives a contribution due to all possible pairings of the instantons. The interaction strength $P(\tau)$ is given by

$$P(\tau) = 2\alpha_c \ln \left| \frac{\theta\omega_d}{\pi} \sin \left[\frac{\pi\tau}{\theta} \right] \right|, \quad (2.23)$$

where α_c is the dimensionless parameter introduced in Eq. (2.6). Since we are rewriting the $2n$ instanton–anti-instanton configuration in terms of a configuration of n extended bounces, we introduce the bounce lengths

$$\tau_j = s_{2j} - s_{2j-1}. \quad (2.24)$$

The bounces are separated by the distances

$$\rho_j = s_{2j+1} - s_{2j}$$

as indicated in Fig. 3. The dissipative portion of the action (2.22) can now be recast as

$$S_d[q(\tau)] = \sum_{j=1}^n S_{B,j}^{\text{self}}(\tau_j) + \sum_{\substack{j,k=1 \\ j < k}}^n \Omega_{jk} \hbar, \quad (2.25)$$

$$S_{B,j}^{\text{self}}(\tau_j) = 2S_I^{\text{self}} + \hbar P(\tau_j).$$

In this expression $S_{B,j}^{\text{self}}$ is the dissipative self-interaction of the j th bounce, it contains the self-interaction of the instanton $2j-1$ and the anti-instanton $2j$, as well as the interaction $\hbar P(\tau_j)$ between this instanton/anti-instanton pair, forming the bounce. Further, we have that

$$\Omega_{j,k} = P(s_{2k} - s_{2j-1}) + P(s_{2k-1} - s_{2j}) - P(s_{2k} - s_{2j}) - P(s_{2k-1} - s_{2j-1}) \quad (2.26)$$

is the interaction between the bounce labeled by j and the bounce labeled by k .

We will show, self-consistently, that in the region of incoherent tunneling the average length of the extended bounce

$$\tau_B = \langle \tau_j \rangle \quad (2.27)$$

is very small compared with their average separation

$$\rho_B = \langle \rho_j \rangle. \quad (2.28)$$

Using the limit that $\rho_j \gg \tau_j$, we may rewrite the inter-bounce interaction as

$$\Omega_{jk} \simeq -2\alpha_c \left[\frac{\pi}{\theta} \right]^2 \sin^{-2} \left[\left[\frac{\pi}{\theta} \right] (s_{2k-1} - s_{2j}) \right] \tau_j \tau_k. \quad (2.29)$$

Hence, in the limit of low temperatures, $\theta \gg \tau_B$, the interaction term Ω_{jk} is at most of order $2\alpha_c (\tau_B / \rho_B)^2$. Thus, provided we can show the inequality

$$\tau_B \ll \rho_B \quad (2.30)$$

is satisfied, the bounces are only weakly interacting at low temperatures and may be treated in the dilute-gas approximation.

This dilute-bounce-gas approximation (DBG) corresponds to formally viewing the instantons and anti-instantons as being charges of opposite sign. This plasma of charges is strongly interacting through the logarithmic coupling mediated by the Ohmic heat bath. As a consequence, the usual dilute instanton gas approximation cannot be applied to the evaluation of the partition function Z_L . However, in the regime of incoherent tunneling, the

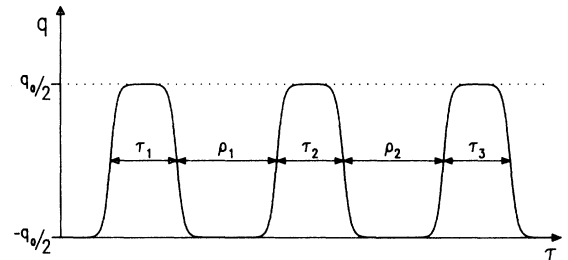


FIG. 3. A typical n -bounce trajectory. The bounce lengths are indicated by τ_i and their separations by ρ_i .

dissipative interaction is strong enough to bind the charges to form dipoles, corresponding to the extended bounces introduced above. The internal interaction within each dipole must be fully taken into account, while the dipoles interact with each other only weakly. As a consequence, the dilute gas approximation is still reasonable if one identifies the molecules of the gas with the extended bounces comprised of the instanton–anti-instanton pairs.

In the DBGA the action associated with the configuration comprised of n extended bounces can be written as

$$S[q(\tau)] = \sum_{j=1}^n S_{B,j}(\tau_j). \quad (2.31)$$

In this expression $S_{B,j}$ is the action due to the bounce labeled by j , including the self-interaction due to the dissipation $S_{B,j}^{\text{self}}$. The partition function Z_L of the metastable state confined to the left well may be written in the form

$$Z_L = \sum_{n=0}^{\infty} z_{L,n}, \quad (2.32)$$

in which $z_{L,0}$ is the contribution from all the trajectories that are entirely confined to the well at $q = -q_0/2$. The terms $z_{L,n}$ represent the contributions from all the trajectories composed of n extended bounce configurations.

The contribution $z_{L,0}$ is determined by the trivial saddle point $q(\tau) = -q_0/2$ in (2.8). A standard calculation gives

$$z_{L,0} = \frac{N}{\left[\prod_{n=0}^{\infty} \Lambda_n^{(0)} \right]^{1/2}} \quad (2.33)$$

where the $\Lambda_n^{(0)}$ are the eigenvalues of the Hermitian eigenvalue equation

$$\left[-M \frac{\partial^2}{\partial \tau^2} + \frac{\partial^2 V}{\partial q^2}(-q_0/2) \right] \varphi_n^{(0)}(\tau) + \int_{-\theta/2}^{\theta/2} d\tau' k(\tau - \tau') \varphi_n^{(0)}(\tau') = \Lambda_n^{(0)} \varphi_n^{(0)}(\tau), \quad (2.34)$$

with periodic boundary conditions and where the constant N has been chosen to make (2.33) agree with the partition function of a damped harmonic oscillator.^{24,27,28} Note that the constant N will cancel in the expression for $\text{Im}F$.

The one-bounce contribution $z_{L,1}$ is the first nontrivial contribution to Z_L . In order to evaluate the functional integral for $z_{L,1}$ we first introduce a bouncelike trajectory $\tilde{q}(\tau; \tau_1, \tau_\phi)$ with period θ , where τ_1 and τ_ϕ characterize the length and the center of the bounce, respectively, and

which extremalizes the action for given parameters τ_1 and θ . Next, the arbitrary path about the bounce is written as

$$q(\tau) = \tilde{q}(\tau; \tau_1, \tau_\phi) + \sum_{n=0}^{\infty} c_n \varphi_n^{(B)}(\tau), \quad (2.35)$$

where the $\varphi_n^{(B)}$ are a complete set of real orthonormal functions with periodic boundary conditions. Further, the $\varphi_n^{(B)}$ are chosen to be eigenfunctions of the second variational derivative of S at \tilde{q}

$$\left[-M \frac{\partial^2}{\partial \tau^2} + V''(\tilde{q}(\tau)) \right] \varphi_n^{(B)}(\tau) + \int_{-\theta/2}^{\theta/2} d\tau' k(\tau - \tau') \varphi_n^{(B)}(\tau') = \Lambda_n^{(B)} \varphi_n^{(B)}(\tau). \quad (2.36)$$

The action corresponding to the arbitrary path (2.35) is then diagonal in the coefficients c_n up to quadratic order

$$S[q(\tau)] = S_{B,1}(\tau_1) + \sum_{n=0}^{\infty} \frac{1}{2} \Lambda_n^{(B)} c_n^2, \quad (2.37)$$

where $S_{B,1}(\tau_1)$ is the action of \tilde{q} . Note that $S_{B,1}$ depends on τ_1 , but is independent of τ_ϕ due to the translational invariance of the action, i.e.,

$$\tilde{q}(\tau; \tau_1, \tau_\phi) = \tilde{q}(\tau - \tau_\phi; \tau_1).$$

The derivative $\partial \tilde{q} / \partial \tau_\phi = -\partial \tilde{q} / \partial \tau$ is then found to be an exact eigenfunction $\varphi_1^{(B)}(\tau)$, with zero eigenvalue $\Lambda_1^{(B)} = 0$. This is a Goldstone type of mode which restores the time translational invariance broken by our choice of the initial phase τ_ϕ of the bounce. Further it will turn out that the bounce action $S_{B,1}(\tau_1)$ shows only a weak dependence on τ_1 . Since the action is roughly invariant under the change

of τ_1 , we find that $\partial \tilde{q} / \partial \tau_1$ is an approximate eigenfunction of the fluctuation spectrum. This eigenfunction represents fluctuations that change the relative separation between the instanton–anti-instanton portions of the extended bounce. This is the so-called “breathing mode.” As we shall see in Sec. IV, this mode corresponds to a small negative eigenvalue, $\Lambda_0^{(B)} < 0$, approaching zero as $\tau_1 \rightarrow \infty$. Thus we obtain for the two lowest normalized eigenfunctions

$$\varphi_0^{(B)}(\tau) = \left[\int_{-\theta/2}^{\theta/2} d\tau' \left[\frac{\partial \tilde{q}}{\partial \tau_1} \right]^2 \right]^{-1/2} \frac{\partial}{\partial \tau_1} \tilde{q}(\tau; \tau_1, \tau_\phi), \quad (2.38)$$

$$\varphi_1^{(B)}(\tau) = \left[\int_{-\theta/2}^{\theta/2} d\tau' \left[\frac{\partial \tilde{q}}{\partial \tau_\phi} \right]^2 \right]^{-1/2} \frac{\partial}{\partial \tau_\phi} \tilde{q}(\tau; \tau_1, \tau_\phi).$$

Now the functional integration in (2.8) is performed by in-

tegration over the expansion coefficients $\{c_n\}$, where we restrict ourselves to the Gaussian approximation (2.37). This approximation, however, breaks down for the c_0 and c_1 integration due to the smallness of the corresponding two eigenvalues $\Lambda_0^{(B)} \lesssim 0$ and $\Lambda_1^{(B)} = 0$. In this case the

$$z_{L,1} = \frac{N}{2\pi\hbar} \int_{-\theta/2}^{\theta/2} d\tau_\phi \int_0^\theta d\tau_1 \exp[-S_{B,1}(\tau_1)/\hbar] \left[\int_{-\theta/2}^{\theta/2} d\tau \left(\frac{\partial \bar{q}(\tau; \tau_1)}{\partial \tau_1} \right)^2 \right]^{1/2} \left[\int_{-\theta/2}^{\theta/2} d\tau' \left(\frac{\partial \bar{q}(\tau'; \tau_1)}{\partial \tau'} \right)^2 \right]^{1/2} \left[\prod_{n=2}^{\infty} \Lambda_n^{(B)} \right]^{-1/2}. \quad (2.39)$$

Due to the translational invariance, the integral over τ_ϕ is trivial, and just produces a factor of θ . The integration over τ_1 is more complicated. The action $S_{B,1}(\tau_1)$ of a bouncelike trajectory mainly depends on τ_1 through two terms. First, τ_1 is the time which the trajectory lingers in the well at $q = +q_0/2$. Since the potential is lower by $-\hbar\sigma$, the action picks up the term $-\hbar\sigma\tau_1$. Secondly, there is the interaction between the instanton and anti-instanton portion of the bounce, described by $\hbar P(\tau_1)$. Thus we write

$$S_{B,1}(\tau_1) = S_{B,1}^{(0)} + \hbar[P(\tau_1) - \sigma\tau_1], \quad (2.40)$$

in which $S_{B,1}^{(0)}$ is the action associated with the two traversals of the barrier. This term $S_{B,1}^{(0)}$ is independent of τ_1 , when $\tau_1 \gg \tau_0$. Note that neither $S_{B,1}^{(0)}$ nor $P(\tau_1)$ are uniquely defined, since a constant term can be shifted between the two parts, merely by changing the arbitrary integration constant ω_d , in (2.20). Since all the other factors in $z_{L,1}$ given in (2.39), have a negligible τ_1 dependence, the τ_1 integral is of the form

$$I_1 = \int_0^\theta d\tau_1 \exp[-S_{B,1}(\tau_1)/\hbar] \simeq \exp(-S_{B,1}^{(0)}/\hbar) \int_0^\theta d\tau_1 \exp[\sigma\tau_1 - P(\tau_1)]. \quad (2.41)$$

$$\text{Im}I_1 = \exp(-S_{B,1}^{(0)}/\hbar) \frac{1}{2i} \left[\int_{\tau_s}^{\tau_s+i\infty} d\tau_1 \exp[\sigma\tau_1 - P(\tau_1)] - \text{c.c.} \right]. \quad (2.43)$$

Now the difference between the τ_1 integral and its complex conjugate may be written as a single integral running from $\tau = \tau_s - i\infty$ up to $\tau = \tau_s + i\infty$. Thus,

$$\text{Im}I_1 = \frac{1}{2} [\exp(-S_{B,1}^{(0)}/\hbar)] K, \quad (2.44)$$

where

$$K = \frac{1}{i} \int_{\tau_s-i\infty}^{\tau_s+i\infty} d\tau_1 \exp[\sigma\tau_1 - P(\tau_1)]. \quad (2.45)$$

We first shift the variable of integration such that it becomes an integration along the imaginary axis. The analytical properties of the integrand allow us to shift the integration contour to slightly positive values. Thus

$$K = \frac{1}{i} \left[\frac{\pi}{\theta\omega_d} \right]^{2\alpha_c} \int_{\epsilon\theta-i\infty}^{\epsilon\theta+i\infty} d\tau_1 \frac{\exp(\sigma\tau_1)}{\sin^{2\alpha_c}(\pi\tau_1/\theta)},$$

standard procedure consists in replacing the integration over c_0 and c_1 by the corresponding integration over the collective coordinates τ_1 and τ_ϕ , respectively. The Jacobian of this transformation can be deferred from (2.35) and (2.38). Thus we find for the single-bounce contribution

For finite temperatures, the integral is convergent. The integrand is largest for values of τ_1 close to the boundaries of integration. The integrand of (2.41) is a minimum at

$$\tau_s = \left[\frac{\theta}{\pi} \right] \text{arccot} \left[\frac{\theta\sigma}{2\pi\alpha_c} \right]. \quad (2.42)$$

At zero temperature, the integral diverges.

As we have previously mentioned, Z_L is the partition function for the metastable well at $q = -q_0/2$. It is written as the functional integral expression, which is to be evaluated only over all the periodic path which mostly remain close to $q = -q_0/2$. This statement can now be made more precisely. The paths for which $\tau_1 > \tau_s$ are to be considered as contributing to Z_R and should be discarded. Only the paths for which $\tau_1 < \tau_s$ contribute to Z_L . Following Langer,¹⁸ we distort the integration contour at τ_s and then continue the integration along the imaginary axis from τ_s to $\tau_s + i\infty$.

Thus the modified integral I_1 acquires an imaginary part given by

which can be written as the sum of the contributions along the positive and negative imaginary axis separately

$$K = \left[\frac{\pi}{\theta\omega_d} \right]^{2\alpha_c} \left[\int_0^\infty dx \frac{\exp(i\sigma x - i\pi\alpha_c)}{\sinh^{2\alpha_c}(\pi x/\theta)} + \text{c.c.} \right]. \quad (2.46)$$

This can be expressed in terms of the β functions yielding the form

$$K = \frac{1}{\omega_d} \left[\frac{2\pi}{\theta\omega_d} \right]^{2\alpha_c-1} \left[\frac{\exp(\theta\sigma/2) |\Gamma(\alpha_c + i\theta\sigma/2\pi)|^2}{\Gamma(2\alpha_c)} \right]. \quad (2.47)$$

Hereby we have rewritten the β function in terms of the Γ functions.⁹

Since the τ_1 dependence of the other quantities in $z_{L,1}$

only gives rise to higher-order corrections, we may evaluate these at the saddle-point value of τ_1 , $\tau_1 = \tau_s$. Thus, the one-bounce contribution to the partition function has an imaginary part given by

$$\text{Im}z_{L,1} = \frac{\theta}{2} z_{L,0} \left[\frac{\Delta}{2} \right]^2 K, \quad (2.48)$$

where we have introduced the dressed tunnel splitting $\Delta/2$ through the relation

$$\frac{\Delta^2}{4} = \omega_0^2 LR \exp(-S_{B,1}^{(0)}/\hbar), \quad (2.49a)$$

where $S_{B,1}^{(0)}$ is defined by Eq. (2.40) and the dimensionless factors L and R are given by

$$L = \frac{M}{2\pi\hbar} \left[\int_{-\theta/2}^{\theta/2} d\tau \left[\frac{\partial \bar{q}(\tau, \tau_s)}{\partial \tau} \right]^2 \right]^{1/2} \\ \times \left[\int_{-\theta/2}^{\theta/2} d\tau \left[\frac{\partial \bar{q}(\tau, \tau_s)}{\partial \tau_s} \right]^2 \right]^{1/2} \quad (2.49b)$$

and

$$R = \frac{1}{M\omega_0^2} \left[\prod_{n=0}^{\infty} \Lambda_n^{(0)} / \prod_{n=2}^{\infty} \Lambda_n^{(B)} \right]^{1/2}. \quad (2.49c)$$

We note that the dominant temperature dependence of $\text{Im}z_{L,1}/\theta$ occurs in the factor K of Eq. (2.45). Thus, the tunnel splitting may be evaluated at $T=0$. The leading corrections to this approximation are of order $(k_B T/\hbar\omega_0)^2$, and so are negligible for $k_B T \ll \hbar\omega_0$.

The above analysis shows that the contributions from the bouncelike trajectories to the partition function Z is well defined as long as $\hbar\beta\sigma = \theta\sigma$ is finite. However, Z is a real quantity and does not contain information about the dynamics of the tunneling decay processes. The partition function of a metastable state is only defined when one restricts the trace to the trace over a subspace of the full Hilbert space. We have evaluated Z_L by excluding the tunneling trajectories that remain near $q = +q_0/2$ for periods longer than τ_s . It should be noted that in the limit $\theta\sigma \rightarrow \infty$, the contributions from the trajectories with $\tau_1 > \tau_s$ would become divergent. We have adapted Langer's method of regularizing divergent partition functions,¹⁸ to the present problem. The contour of integration over τ_1 has been distorted at τ_s to run into the upper half of the complex plane. In the limit $\theta \rightarrow \infty$, this is just the usual procedure, as formulated by Langer.¹⁸

The one-bounce contribution to the partition function $z_{L,1}$ contains the factor Δ^2 and thus represents an exponentially small correction to $z_{L,0}$. This correction is only kept, in this semiclassical approximation, since it gives the leading imaginary component to Z_L .

It can be easily shown that the n -bounce contributions $z_{L,n}$ only gives a correction of order Δ^{2n} . Thus, the dominant part of Z_L is that contained in $z_{L,1}$.

Using the definition

$$Z_L = z_{L,0} \left[1 + \sum_{n=1}^{\infty} z_{L,n}/z_{L,0} \right] \quad (2.50)$$

and

$$F_L = -\frac{1}{\beta} \ln Z_L \quad (2.51)$$

we find that the free energy has an imaginary part. To leading order, we have

$$\text{Im}F_L = -\frac{1}{\beta} \text{Im} \ln(1 + z_{L,1}/z_{L,0}), \quad (2.52)$$

and since the factor $z_{L,1}/z_{L,0}$ is exponentially small, the logarithm can be expanded, yielding

$$\text{Im}F_L = -\frac{\hbar}{2} \left[\frac{\Delta}{2} \right]^2 K. \quad (2.53)$$

This imaginary part of the free energy is to be interpreted as the imaginary component of a resonance energy in quantum field theory. That is, it describes the rate of transitions out of the metastable state.¹⁸ Thus, we have the rate of tunneling transitions out of the left well, given by

$$\Gamma^+ = -\frac{2}{\hbar} \text{Im}F_L = \left[\frac{\Delta}{2} \right]^2 K. \quad (2.54)$$

Inserting Eqs. (2.47) and (2.49) we obtain

$$\Gamma^+ = \frac{\omega_0^2}{\omega_d} LR \left[\frac{2\pi}{\theta\omega_d} \right]^{2\alpha_c - 1} \frac{\left| \Gamma \left[\alpha_c + \frac{i\theta\sigma}{2\pi} \right] \right|^2}{\Gamma(2\alpha_c)} \\ \times \exp \left[\frac{\theta\sigma}{2} \right] \exp(-S_{B,1}^{(0)}/\hbar). \quad (2.55)$$

We note that the above expression is actually independent of the arbitrary frequency scale ω_d . A shift of $\omega_d \rightarrow \xi\omega_d$ would result in a change $S_{B,1}^{(0)}$ by the additive term $-2\alpha_c \hbar \ln \xi$ which exactly cancels with the factor occurring in the first two terms of (2.55). Thus Eq. (2.55) is independent of the choice of ω_d . We shall, henceforth, put $\omega_d = \omega_0$.

Having found the expression for Γ^+ , we are now able to check the consistency of the dilute-bounce-gas approximation. Since the typical bounce length is given by $\tau_s \simeq \tau_B$, and the typical bounce separation $\rho_B \simeq \Gamma^{-1}$ the self-consistency condition (2.30) reduces to

$$\tau_s \Gamma^+ \ll 1.$$

Since Γ^+ is of order Δ^2 , the above condition is generally satisfied, except at very low temperatures where τ_s may diverge. Since τ_s is proportional to θ and Γ^+ is proportional to $\theta^{1-2\alpha_c}$, at low temperatures and for $\sigma=0$, we find that $\tau_s \Gamma^+$ is proportional to $\theta^{2(1-\alpha_c)}$. This shows that the inequality may hold for $\sigma=0$, even in the limit $T \rightarrow 0$, if $\alpha_c > 1$. For finite bias σ , τ_s is finite even at zero temperature, and the range of validity of the DBGGA is much larger.

In complete analogy with the above reasoning, one can calculate the rate of tunneling transitions out of the well at $q = +q_0/2$. The only difference in the final formula is

that $z_{L,0}$ is replaced by $z_{R,0}=z_{L,0}\exp(\theta\sigma)$, due to the bias.

The imaginary parts $\text{Im}z_{R,1}=-\text{Im}z_{L,1}$, since the total partition function is real, and both contributions arise from a distortion of the contour into the upper half τ_1 plane. Thus we obtain

$$\Gamma^- = \Gamma^+ \exp(-\theta\sigma). \quad (2.56)$$

Thus Γ^+ and Γ^- obey the principle of detailed balance. This concludes our derivation of the general formula for the rate of incoherent tunneling between the minima of the damped double-well system.

III. CALCULATIONS OF THE EXTREMAL TRAJECTORIES FOR A MODEL POTENTIAL

In this section, we illustrate for $T=0$ the general theory developed in Sec. II with the explicit calculations for a model potential $V(q)$. The specific form of $V(q)$ is given by

$$V(q) = \begin{cases} \frac{M}{2} \omega_0^2 (q + q_0/2)^2, & q < q_m \\ \frac{M}{2} \omega_0^2 (q - q_0/2)^2 - \hbar\sigma, & q > q_m \end{cases} \quad (3.1a)$$

$$(3.1b)$$

The point q_m is the position of the maximum of the potential barrier; it is related to the bias σ through

$$q_m = -\frac{\hbar\sigma}{8V_0} q_0, \quad (3.2)$$

where V_0 is the height of the potential barrier in the unbiased case ($\sigma=0$). The parameter V_0 is given by

$$V_0 = \frac{1}{8} M \omega_0^2 q_0^2. \quad (3.3)$$

The potential is sketched in Fig. 4. The barrier height V_m , of the biased potential is given by the expression

$$V_m = V(q_m) = V_0 \left[1 - \frac{1}{2} \left(\frac{\hbar\sigma}{V_0} \right) + \frac{1}{16} \left(\frac{\hbar\sigma}{V_0} \right)^2 \right]. \quad (3.4)$$

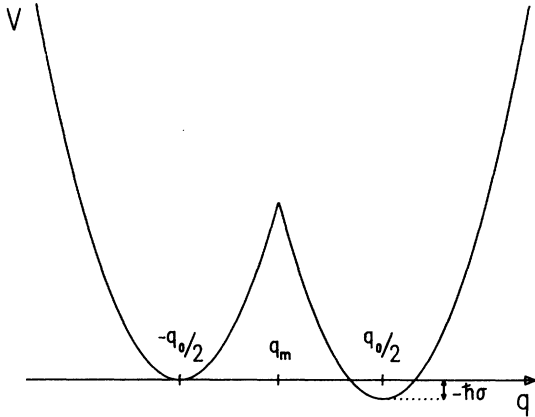


FIG. 4. The asymmetric double-well potential $V(q)$ described in equation (3.1). The maximum of the potential barrier is located at q_m .

We shall determine the paths which extremalize the action (2.9), for this particular potential. The extremal paths obey the Euler-Lagrange equation (2.15). As mentioned previously, in Sec. II, these paths as well as their neighboring paths dominate the dynamics of the decay process. In particular, we shall consider bouncelike paths, $\tilde{q}(\tau)$, consisting of instanton-anti-instanton pairs separated by a time τ_1 . This is to allow us to explicitly consider the effect of the “breathing” mode beyond the Gaussian approximation. The particular choice of this family of trajectories are those which satisfy the equation of motion (2.15) at all times, except at the isolated points $\tau = \pm\tau_1/2$. At these points the instanton trajectory reaches q_m where the potential has a cusp. At the cusp, we introduce a discontinuous jump in the velocity

$$\lambda \equiv \dot{q}(\tau_1/2 - 0) - \dot{q}(\tau_1/2 + 0). \quad (3.5)$$

A typical member of this family of trajectories is depicted in Fig. 5. The class of bouncelike trajectories $q(\tau)$ obeys the equation of motion

$$-\ddot{\tilde{q}}(\tau) + \frac{1}{M} \int_{-\infty}^{\infty} d\tau' k(\tau - \tau') \tilde{q}(\tau') + \frac{1}{M} \frac{\partial}{\partial \tilde{q}} V(\tilde{q}) = \lambda [\delta(\tau - \tau_1/2) + \delta(\tau + \tau_1/2)], \quad (3.6)$$

where λ is defined in Eq. (3.5). These trajectories satisfy the boundary conditions $\tilde{q}(\tau \rightarrow \pm\infty) = -q_0/2$. In the above equation, and in what follows we have taken the zero-temperature limit, i.e., $\theta \rightarrow \infty$.

The bounce trajectory, which extremalizes the action, is contained within this class and corresponds to the trajectory for which $\lambda=0$. We shall denote the value of τ_1 that is associated with this particular trajectory as τ_s . The equation of motion (3.6), is readily solved by the use of the Fourier transform

$$\tilde{q}(\tau) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega Q(\omega) \exp(i\omega\tau). \quad (3.7)$$

Using Eq. (2.12), we obtain from the Fourier transform of Eq. (3.6), the expression for the Fourier amplitude $Q(\omega)$;

$$Q(\omega) = \frac{1}{\omega^2 + \xi(\omega) + \omega_0^2} \left[\frac{\omega_0^2}{2} q_0 \left[4 \frac{\sin(\omega\tau_1/2)}{\omega} - 2\pi\delta(\omega) \right] + 2\lambda \cos \left[\frac{\omega\tau_1}{2} \right] \right], \quad (3.8)$$

in which $\xi(\omega) = |\omega| \tilde{\gamma}(\omega)$ as in Eq. (2.14). In deriving (3.8), we have made explicit use of the expression for the derivative of the potential

$$\frac{1}{M} \frac{\partial V}{\partial q} = \omega_0^2 q - \frac{1}{2} q_0 \omega_0^2 \epsilon(\tau), \quad (3.9)$$

where

$$\epsilon(\tau) = \begin{cases} +1, & |\tau| < \tau_1/2 \\ -1, & |\tau| > \tau_1/2 \end{cases}.$$

Thus, the explicit form of the bouncelike trajectory, obeying (3.6), is given by

$$\begin{aligned} \tilde{q}(\tau) + q_0/2 = & q_0 \omega_0^2 \frac{2}{\pi} \int_0^\infty d\omega \frac{\sin(\omega\tau_1/2)\cos(\omega\tau)}{\omega[\omega^2 + \xi(\omega) + \omega_0^2]} \\ & + \lambda \frac{2}{\pi} \int_0^\infty d\omega \frac{\cos(\omega\tau_1/2)\cos(\omega\tau)}{[\omega^2 + \xi(\omega) + \omega_0^2]}. \end{aligned} \quad (3.10)$$

The parameter λ determining the discontinuity in the velocity (3.5) is found to be

$$\lambda = \omega_0 \left[\frac{q_0[1 - K_1(\tau_1/2)] + 2q_m}{2K_+(\tau_1/2)} \right], \quad (3.11)$$

where the functions K_1 and K_+ are defined in the Appendix.

The bounce trajectory $q_B(\tau)$, follows from the expression (3.10), by setting $\tau_1 = \tau_s$, at which point $\lambda = 0$. Thus, we find the bounce trajectory as

$$q_B(\tau) + q_0/2 = q_0/2 \left[K_1 \left[\frac{\tau_s}{4} + \frac{\tau}{2} \right] + K_1 \left[\frac{\tau_s}{4} - \frac{\tau}{2} \right] \right] \quad (3.12)$$

(see Fig. 5). The bounce time τ_s is determined from Eq. (3.11), with $\lambda = 0$. In the case of Ohmic damping, defined by $\xi(\omega) = \gamma |\omega|$, one can determine τ_s from the asymptotic behavior of K_1 , given in Eq. (A7) of the Appendix. The result is given by

$$\omega_0 \tau_s = \frac{2q_0 \alpha}{\pi |q_m|} = \frac{16V_0 \alpha}{\pi \hbar |\sigma|}, \quad \omega_0 \tau_s \gg 1, \quad (3.13)$$

where α is defined by

$$\alpha = \frac{\gamma}{2\omega_0} \quad (3.14)$$

as the dimensionless strength of the damping mechanism. In deriving the bounce time τ_s , we have assumed that $\omega_0 \tau_s \gg 1$.

The asymptotic long-time behavior of the bounce trajectory shows the characteristic $1/\tau^2$ variation expected for Ohmic dissipation. As discussed in Sec. II, this behavior ensures that the asymptotic part of the action defined in Eq. (2.19), remains finite. This can be readily established, by examining the behavior of (3.12) in the Ohmic case. We find

$$q_B(\tau) + \frac{q_0}{2} = q_0 \left[\frac{2\alpha}{\pi\omega_0} \frac{\tau_s}{\tau^2} + O\left(\frac{1}{\tau^4}\right) \right], \quad \tau \gg \tau_s, \quad (3.15)$$

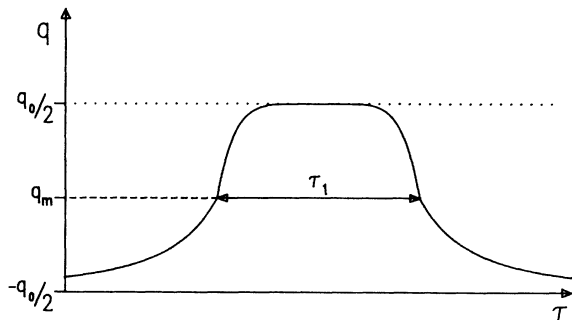


FIG. 5. A sketch of a bouncelike trajectory (3.10), for a general value of τ_1 , given by Eq. (3.11).

where we have utilized the asymptotic behavior of the functions K_1 discussed in the Appendix. [Note that $K_1(\tau)$ is an odd function of τ .]

A. The action

Using the equation of motion (3.6) the action (2.9) becomes

$$S(\tilde{q}(\tau)) = \int_{-\infty}^{\infty} d\tau \left[V(\tilde{q}(\tau)) - \frac{1}{2} \tilde{q}(\tau) \frac{\partial V}{\partial \tilde{q}(\tau)} \right] + M\lambda q_m. \quad (3.16)$$

On substituting the form of the potential (3.1), we obtain for the action

$$\begin{aligned} S[\tau_1] = & \frac{M\omega_0^2 q_0}{2} \int_0^{\tau_1/2} d\tau \left[\frac{1}{2} q_0 - \tilde{q}(\tau) \right] \\ & + \frac{M\omega_0^2}{2} q_0 \int_{\tau_1/2}^{\infty} d\tau \left[\frac{1}{2} q_0 + \tilde{q}(\tau) \right] \\ & - \hbar \sigma \tau_1 + M\lambda q_m, \end{aligned} \quad (3.17)$$

where we have explicitly shown the τ_1 dependence.

On using the form of $\tilde{q}(\tau)$ given in Eq. (3.10), this can be written in terms of the K functions defined in the Appendix as

$$\begin{aligned} S[\tau_1] = & M\omega_0 q_0^2 \left[K_- \left[\frac{\tau_1}{2} \right] + K_2 \left[\frac{\tau_1}{2} \right] \right] - \hbar \sigma \tau_1 \\ & + M\lambda \left\{ \frac{q_0}{2} \left[1 - K_1 \left[\frac{\tau_1}{2} \right] \right] + q_m \right\} \end{aligned} \quad (3.18)$$

being valid for arbitrary damping mechanisms $\xi(\omega)$, and arbitrary τ_1 . The action $S[\tau_1]$, for the family of trajectories, is an extremum at the value $\tau_1 = \tau_s$, $S[\tau_1 = \tau_s] \equiv S_{\text{ex}}[\tau_s]$. At the extremal point $\tau_1 = \tau_s$ the velocity jump (3.11) vanishes, and $\lambda(\tau_s) = 0$. In the case of Ohmic dissipation, the extremal action associated with this bounce trajectory is given by

$$\begin{aligned} S_{\text{ex}}[\tau_s]/\hbar = & 2\alpha_c [C + \ln(\omega_0 \tau_s)] - \sigma \tau_s \\ & + \frac{4V_0}{\hbar\omega_0} (1 - 2\alpha^2) s(\alpha) + O(1/\omega_0^2 \tau_s^2), \end{aligned} \quad (3.19)$$

where we have used the asymptotic form $\omega_0 \tau_s \gg 1$ of the K_n functions, as given in the Appendix. In the above expression $C = 0.5772\dots$ is Euler's constant and $s(\alpha)$ is given by Eq. (A4), i.e.,

$$s(\alpha) = \frac{1}{\pi(\alpha^2 - 1)^{1/2}} \ln \left[\frac{\alpha + (\alpha^2 - 1)^{1/2}}{\alpha - (\alpha^2 - 1)^{1/2}} \right].$$

The parameter $\alpha_c = 8V_0 \alpha / \pi \hbar \omega_0$ is the same as that previously defined in Eq. (2.6). We note the relation between the functions $s(\alpha)$ and the mean-square displacement of the damped harmonic oscillator

$$\langle q^2 \rangle = \frac{\hbar}{2m\omega_0} s(\alpha)$$

derived in Refs. 27 and 28. Following Eq. (2.40), we split

the extremal action into three parts

$$S_{\text{ex}}[\tau_s] \equiv S_{B,1} = S_{B,1}^{(0)} + \hbar P(\tau_s) - \hbar \sigma \tau_s,$$

where

$$P(\tau_s) = 2\alpha_c \ln(\omega_0 \tau_s). \quad (3.20a)$$

The first term $S_{B,1}^{(0)}$ is the action corresponding to the instanton–anti-instanton pair, without their mutual interactions. $S_{B,1}^{(0)}$ is given by

$$S_{B,1}^{(0)}/\hbar = 2 \left[\alpha_c C + \frac{2V_0}{\hbar\omega_0} (1 - 2\alpha^2) s(\alpha) + O(1/\omega_0^2 \tau_s^2) \right]. \quad (3.20b)$$

The second term in Eq. (3.20) describes the interaction between the instanton and anti-instanton parts of the bounce. The last term is due to the bias. The action (3.20) simplifies in the limit of very large α , $\alpha \gg 1$. The limiting behavior of the action may be obtained with the aid of the asymptotic form of $s(\alpha)$

$$\lim_{\alpha \rightarrow \infty} s(\alpha) = \frac{2}{\pi\alpha} \left[\ln(2\alpha) \left[1 + \frac{1}{2\alpha^2} \right] - \frac{1}{4\alpha^2} + O(\alpha^{-4}) \right]. \quad (3.21)$$

Thus, we obtain the asymptotic large α behavior of the bounce action as

$$S_{\text{ex}}[\tau_s]/\hbar = 2\alpha_c \ln(\omega_0 \tau_s) - \sigma \tau_s - 2\alpha_c \left[\ln(\alpha_c) - \ln \left[\frac{8V_0}{\hbar\omega_0} \right] + c_\infty \right], \quad \alpha \gg 1, \quad (3.22)$$

where the constant $c_\infty = \ln(2\pi) - C = 1.2606 \dots$. The action can be rewritten as

$$S_{\text{ex}}[\tau_s]/\hbar = 2\alpha_c \left[\ln \left[\frac{16V_0}{h\sigma} \right] - 1 - c_\infty \right], \quad \alpha \gg 1. \quad (3.23)$$

In obtaining this expression, we have used the formula for the bounce time τ_s given in (3.13).

In this section we have, thus far, restricted our attention to the case of zero temperature. At finite temperatures, we again obtain an expression of the form of (3.18), where the integrals in (A1) defining the functions K_1 , K_2 , and K_\pm are replaced by the corresponding Fourier sums. On neglecting terms of order $(\omega_0 \theta)^{-2}$ we obtain $S_{\text{ex}}(\tau_s)$ in the form (3.20), where $P(\tau_s)$ is given by the expression (2.23) with $\omega_d = \omega_0$. We note that the expression (3.20) is exactly in the form of (2.40), which was used in Sec. II.

B. The energy loss

We shall now evaluate the energy loss associated with the zero-temperature bounce trajectory. The extremal bounce may be conceptually decomposed into an instanton–anti-instanton pair. The instanton trajectory starts at the point $q = -q_0/2$ and ends up at the point

$\bar{q} = q_B(0)$ at time $\tau = 0$. The exit point \bar{q} is evaluated from Eq. (3.12) as

$$\bar{q} = -q_0/2 + q_0 K_1 \left[\frac{\tau_s}{4} \right]. \quad (3.24)$$

On using the asymptotic expansion ($\omega_0 \tau \gg 1$) of K_1 , found in the Appendix, we find

$$\bar{q} = q_0 \left[\frac{1}{2} - \frac{8\alpha}{\pi\omega_0 \tau_s} \right] = \frac{1}{2} q_0 \left[1 - \frac{\hbar\sigma}{V_0} \right]. \quad (3.25)$$

Since the kinetic energy vanishes at both the turning points, the energy loss over the instanton part of the bounce is associated with the difference of the potential energy at these turning points. As we have defined $V(-q_0/2) = 0$, the energy loss ΔE emerges as

$$\Delta E = -V(\bar{q}) = \hbar\sigma \left[1 - \frac{\hbar\sigma}{V_0} \right]. \quad (3.26)$$

This result precisely agrees with the analysis of Weiss *et al.*,⁷ who have considered a more general form of a metastable potential well.

IV. EVALUATION OF THE PREFACTOR OF THE DRESSED TUNNEL MATRIX

The contribution to the path integral from trajectories that describe fluctuations about the bounce determine the preexponential factor $\Omega(\alpha)$ of the tunnel matrix $\Delta/2$ in (2.49):

$$\Omega(\alpha) = \omega_0 \sqrt{L(\alpha)R(\alpha)}. \quad (4.1)$$

In this section we calculate this prefactor for the model potential (3.1) for $T = 0$. We shall find an analytic expression for arbitrary length τ_s of the bounce. Eventually, we shall consider the case of an extended bounce for which the prefactor factorizes into the contributions from the instanton and anti-instanton, respectively.

An arbitrary trajectory close to the bounce trajectory $q_B(\tau) = \bar{q}(\tau - \tau_\phi; \tau_1 = \tau_s)$ can be expanded in terms of a complete set of functions $\varphi_n^{(B)}(\tau)$ [see (2.35)].

In Sec. II we have treated both the translation mode $\varphi_1^{(B)}(\tau)$ and the “breathing” mode $\varphi_0^{(B)}(\tau)$ by going beyond the Gaussian approximation, which was used to treat the other modes. This was achieved by transforming to the collective coordinates τ_ϕ and τ_1 associated with these modes. The integration over τ_1 is given in Eq. (2.41). Since the dominant contributions come from the region $\tau_1 \approx \tau_s$, it is consistent to evaluate the prefactor $\Omega(\alpha)$ for the extremal path $q_B(\tau)$.

The factor $L(\alpha)$ in (4.1) arises from the appropriate normalization of the modes $\varphi_0^{(B)}(\tau)$ and $\varphi_1^{(B)}(\tau)$. This factor can be calculated explicitly for our model potential (3.1). By inserting the bounce solution (3.12) into (2.49) we find

$$L(\alpha) = \frac{M\omega_0 q_0^2}{8\pi\hbar} [\mathcal{J}_+(\tau_s) \mathcal{J}_-(\tau_s)]^{1/2}, \quad (4.2)$$

where the functions $\mathcal{J}_\pm(\tau)$ are discussed in the Appendix. For Ohmic dissipation and in the limit of a large separa-

tion of the instanton–anti-instanton pair forming the bounce we find

$$L(\alpha) = \frac{M\omega_0 q_0^2}{8\pi\hbar} u(\alpha), \quad (4.3)$$

where the function $u(\alpha)$ is defined in (A10), and where terms of order $(\omega_0\tau_s)^{-4}$ have been neglected. The function $u(\alpha)$ behaves as $u(\alpha) = 1 - 4\alpha/\pi + O(\alpha^2)$ in the limit $\alpha \rightarrow 0$ and it vanishes as $1/\alpha$ in the limit $\alpha \rightarrow \infty$,

$$u(\alpha) = \frac{2}{\pi} \frac{1}{\alpha}, \quad \alpha \gg 1. \quad (4.4)$$

Next we turn to the factor $R(\alpha)$ in the expression (4.1). The factor $R(\alpha)$ is defined in (2.49). This factor arises from the contribution of the modes $\varphi_n^{(B)}(\tau)$ about the bounce $q_B(\tau)$ for $n \geq 2$ relative to the modes $\varphi_m^{(0)}(\tau)$, $m \geq 0$, about the trivial path $q(\tau) = -q_0/2$. The product of the eigenvalues in Eq. (2.49c) can be written in the form of an exponential. First, we shall consider the contributions from the Gaussian fluctuations about the bounce, which are

$$\begin{aligned} \left[\prod_{n=2}^{\infty} \Lambda_n^{(B)} \right]^{-1/2} &= \exp \left[-\frac{1}{2} \sum_{n=2}^{\infty} \ln \Lambda_n^{(B)} \right] \\ &= \exp \left[-\frac{1}{2} \int_{M\omega_0^2}^{\infty} d\Lambda \rho_B(\Lambda) \ln \Lambda \right], \end{aligned} \quad (4.5)$$

$$R = \frac{1}{M\omega_0^2} \exp \left[\frac{1}{2\pi} \int_{M\omega_0^2}^{\infty} d\Lambda \int_{-\infty}^{\infty} d\omega \operatorname{Im} \left[T_{\Lambda}(\omega, \omega) \frac{\partial}{\partial \Lambda} \tilde{g}_{\Lambda}(\omega) \right] \ln \Lambda \right], \quad (4.8)$$

where the T matrix is defined by the relation

$$\begin{aligned} \tilde{G}_{\Lambda}(\omega, \omega') &= \tilde{g}_{\Lambda}(\omega) \delta(\omega - \omega') \\ &\quad - \tilde{g}_{\Lambda}(\omega) T_{\Lambda}(\omega, \omega') \tilde{g}_{\Lambda}(\omega'), \end{aligned} \quad (4.9)$$

and \tilde{g}_{Λ} is given by

$$\tilde{g}_{\Lambda}(\omega) = \frac{1}{M[\omega_0^2 + \omega^2 + \xi(\omega)] - \Lambda - i\epsilon}. \quad (4.10)$$

In the specific case under consideration, we find that

$$\begin{aligned} V''(q_B(\tau)) - V''(\pm q_0/2) &= -M\omega_0^2 q_0 \delta(q_B(\tau)) \\ &= -U[\delta(\tau + \tau_s/2) \\ &\quad + \delta(\tau - \tau_s/2)]. \end{aligned} \quad (4.11)$$

Thus, the net potential described by (4.11) consists of two Dirac δ functions, at times $\pm\tau_s/2$, where the inverse strength U^{-1} of the potential is given by

$$U^{-1} = \frac{|\dot{q}_B(\tau_s/2)|}{M\omega_0^2 q_0} = \frac{K_-(\tau_s/2)}{M\omega_0}. \quad (4.12)$$

In deriving the expression for U we have made use of Eq. (3.12) and of the function $K_-(\tau)$ defined in the Appendix. It is important to note that (4.12) can be rewritten in the form

$$U^{-1} = g_{\Lambda=0}(\tau=0) - g_{\Lambda=0}(\tau=\tau_s). \quad (4.13)$$

where in the second line we have transformed to the continuum limit. The continuum spectrum of the eigenvalues has a lower bound which is at $M\omega_0^2$. This latter expression can be evaluated in terms of the Green's function²⁹ defined by

$$\begin{aligned} \left[-M \frac{\partial^2}{\partial \tau^2} + V''(q_B(\tau)) - \Lambda \right] G_{\Lambda}(\tau, \tau'') \\ + \int_{-\infty}^{\infty} d\tau' k(\tau - \tau') G_{\Lambda}(\tau', \tau'') = \delta(\tau - \tau''). \end{aligned} \quad (4.6)$$

The density of eigenvalues $\rho_B(\Lambda)$ is given through the relation

$$\rho_B(\Lambda) = \frac{1}{\pi} \operatorname{Im} \int_{-\infty}^{\infty} d\omega \tilde{G}_{\Lambda}(\omega, \omega), \quad (4.7)$$

where $\tilde{G}_{\Lambda}(\omega, \omega')$ denotes the Fourier transform of the Green's function $G_{\Lambda}(\tau, \tau')$.

Since the same manipulations can be performed with the product $\Lambda_n^{(0)}$ we find that the ratio of the products in R merely involve the change in the spectral density caused by the presence of the "potential:" $V''(q_B(\tau)) - V''(\pm q_0/2)$. The dimensionless ratio of the determinants can be expressed as^{29,30}

Here, $g_{\Lambda}(\tau)$ is the Green's function in the absence of the potential

$$\begin{aligned} g_{\Lambda}(\tau) &\equiv g'_{\Lambda}(\tau) + i g''_{\Lambda}(\tau) \\ &= \frac{1}{\pi} \int_0^{\infty} d\omega \frac{\cos(\omega\tau)}{M[\omega^2 + \xi(\omega) + \omega_0^2] - \Lambda - i\epsilon}. \end{aligned} \quad (4.14)$$

A. Evaluation of the T matrix

The T matrix occurring in Eq. (4.8) can be found by solving the equation of motion for the Green's function $G_{\Lambda}(\tau, \tau')$. The Lippmann-Schwinger equation relating $G_{\Lambda}(\tau, \tau')$ to $g_{\Lambda}(\tau - \tau')$ can be rewritten as

$$\begin{aligned} G_{\Lambda}(\tau, \tau'') &= g_{\Lambda}(\tau - \tau'') + U g_{\Lambda}(\tau - \frac{1}{2}\tau_s) G_{\Lambda} \left[\frac{\tau_s}{2}, \tau'' \right] \\ &\quad + U g_{\Lambda}(\tau + \frac{1}{2}\tau_s) G_{\Lambda} \left[\frac{-\tau_s}{2}, \tau'' \right]. \end{aligned} \quad (4.15)$$

On substituting $\tau = \pm \frac{1}{2}\tau_s$ in the above equation we obtain two simultaneous equations linear in $G_{\Lambda}(\pm \frac{1}{2}\tau_s, \tau'')$. Solving these equations and resubstituting back into Eq. (4.15) one finds the exact expression for $G_{\Lambda}(\tau, \tau'')$. The T matrix is then obtained by Fourier transforming the resulting expression for $G_{\Lambda}(\tau, \tau'')$ and comparing with the expres-

sion (4.9). The T matrix is found to be given by the exact expression

$$T_{\Lambda}(\omega, \omega') = \frac{1}{\pi} \frac{1}{N_{+}(\Lambda)N_{-}(\Lambda)} \times \{ (U^{-1} - g_{\Lambda}^{(0)}) \cos[(\omega - \omega')\frac{1}{2}\tau_s] + g_{\Lambda}(\tau_s) \cos[(\omega + \omega')\frac{1}{2}\tau_s] \}, \quad (4.16)$$

where

$$N_{\pm}(\Lambda) = U^{-1} - [g_{\Lambda}(\tau=0) \pm g_{\Lambda}(\tau=\tau_s)], \quad (4.17)$$

and where $g_{\Lambda}(\tau)$ is defined in (4.14). The isolated poles of the T matrix identify the eigenvalues of the bound states which are obtained from the zeros of the functions $N_{\pm}(\Lambda)$. On recalling the expression (4.13) for U^{-1} we immediately recover the zero eigenvalue $\Lambda_1^{(B)} = 0$ from the condition $N_{-}(\Lambda) = 0$.

The equation $N_{+}(\Lambda) = 0$ determines the negative eigenvalue $\Lambda_0^{(B)} < 0$ of the breathing mode previously discussed. For Ohmic dissipation the bound-state condition can be evaluated explicitly in terms of the functions defined in the Appendix. For an extended bounce, where Eq. (3.13) holds, the eigenvalue $\Lambda_0^{(B)}$ approaches zero from below as

$$\Lambda_0^{(B)} = \frac{-16}{\pi} \frac{\alpha}{u(\alpha)} M \omega_0^2 \left[\frac{1}{\omega_0 \tau_s} \right]^2, \quad (4.18)$$

where terms of order $(\omega_0 \tau_s)^{-4}$ have been neglected. Clearly, in the limit $\tau_s \rightarrow \infty$ the instanton–anti-instanton pair regain their independent time translational invariance.

B. The ratio of determinants

The dimensionless ratio R of the determinants can be found from (4.8) by virtue of the explicit expressions (4.16) and (4.10) for $T_{\Lambda}(\omega, \omega)$ and $\tilde{g}_{\Lambda}(\omega)$. Performing the integral over ω we obtain the exponent as

$$\ln(M \omega_0^2 R) = - \int_{M \omega_0^2}^{\infty} \frac{d\Lambda}{2\pi} (\ln \Lambda) \text{Im} \left[\frac{\partial}{\partial \Lambda} \ln [N_{+}(\Lambda) N_{-}(\Lambda)] \right]. \quad (4.19)$$

In deriving this, we have recognized the resulting integrand as a logarithmic derivative. Now, it is convenient to introduce the phase shifts $\delta_{\pm}(\Lambda)$ of the even and odd scattering wave functions, respectively,

$$\delta_{\pm}(\Lambda) = \text{Im} \ln N_{\pm}(\Lambda) = \text{arccot} \left[\frac{U^{-1} - [g'_{\Lambda}(0) \pm g'_{\Lambda}(\tau_s)]}{g''_{\Lambda}(0) \pm g''_{\Lambda}(\tau_s)} \right], \quad (4.20)$$

where in the second line we have used Eqs. (4.17) and (4.14). On performing a partial integration in the resulting expression for R we obtain

$$R = \exp \left[\frac{1}{2\pi} \int_{M \omega_0^2}^{\infty} \frac{d\Lambda}{\Lambda} [\delta_{+}(\Lambda) + \delta_{-}(\Lambda)] \right], \quad (4.21)$$

where the annoying factor $1/M\omega_0^2$ has canceled with the boundary term of the partial integration. This cancellation occurs since the phase shifts satisfy the relation $\delta_{\pm} = \pi$ at the boundary, in accordance with Levinson's theorem. Physically, this is due to the fact that the bounce produces one even and one odd bound state in its fluctuation spectrum and, since the total number of modes is conserved, the continuum must contain two less modes.

The result (4.21), for the ratio of the eigenvalues, is valid for arbitrary dissipation mechanisms $\xi(\omega)$. For the Ohmic case, the real and imaginary parts of the Green's function are given by

$$g'_{\Lambda}(\tau) = \frac{1}{\pi M(\nu_1 + \nu_2)} [g(\nu_1 \tau) - g(\nu_2 \tau) - \pi \sin(\nu_1 \tau)], \quad (4.22)$$

$$g''_{\Lambda}(\tau) = \frac{1}{M(\nu_1 + \nu_2)} \cos(\nu_1 \tau),$$

where

$$\nu_{1/2} = (\alpha^2 \omega_0^2 + \Lambda/M - \omega_0^2)^{1/2} \mp \alpha \omega_0, \quad (4.23)$$

and where $g(z)$ is an auxiliary exponential integral function.³¹ Equations (4.20)–(4.23) give the exact ratio R of the continuous eigenvalues, for arbitrary length τ_s of the bounce. For an extended bounce, where $\omega_0 \tau_s \gg 1$, the nonoscillatory terms of $g'_{\Lambda}(\tau_s)$ are of order $(\omega_0 \tau_s)^{-2}$. Also, the contributions of the oscillatory terms to the integral in (4.21) are only of order $(\omega_0 \tau_s)^{-2}$. Hence, for an extended bounce, $\omega_0 \tau_s \gg 1$, the function $R(\alpha, \tau_s)$ factorizes into two identical terms arising from the fluctuation modes about the isolated instanton and anti-instanton, respectively. We find

$$R = \exp \left[\frac{1}{\pi} \int_{M \omega_0^2}^{\infty} d\Lambda \frac{\delta(\Lambda)}{\Lambda} \right], \quad (4.24)$$

where

$$\delta(\Lambda) = \text{arccot} \left[\frac{U^{-1} - g'_{\Lambda}(\tau=0)}{g''_{\Lambda}(\tau=0)} \right] \quad (4.25)$$

is the phase shift appropriate to the scattering from the potential $-U\delta(\tau)$ of an isolated instanton. On introducing the dimensionless momentum variable p by the relation $\Lambda = M\omega_0^2(1+p^2)$ we find the final form

$$R(\alpha) = \exp \left\{ \frac{2}{\pi} \int_0^{\infty} dp \frac{p}{1+p^2} \text{arccot} \left[s(\alpha)(\alpha^2 + p^2)^{1/2} - \frac{2}{\pi} \text{arcsinh} \left[\frac{\alpha}{p} \right] \right] \right\}, \quad (4.26)$$

where $s(\alpha)$ is defined in (A4). This integration can be performed analytically in the limit of zero dissipation ($\alpha=0$), yielding

$$R(\alpha=0) = 2. \quad (4.27)$$

In the limit of large damping strengths, $\alpha \gg 1$, we find

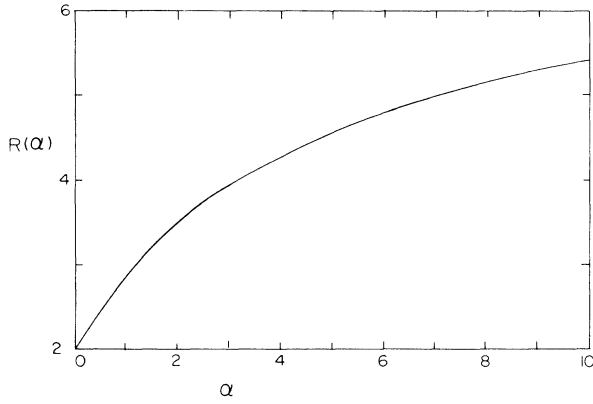


FIG. 6. The α dependence of the ratio of the continuum eigenvalues, $R(\alpha)$, of Eq. (4.26).

$$\begin{aligned} R(\alpha) &= \exp[\ln(\ln\alpha) + 0.714 + O(1/\ln\alpha)] \\ &= 2.042 \ln\alpha [1 + O(1/\ln\alpha)], \end{aligned} \quad (4.28)$$

where the constant has been determined numerically. The function $R(\alpha)$ is plotted, in Fig. 6, as a function of the dissipation parameter α .

On collecting together the factors associated with a single instanton like traversal of the classically forbidden region, we obtain the dressed tunnel matrix element $\Delta/2$ as

$$\frac{\Delta}{2} = \omega_0 \left[\frac{M\omega_0 q_0^2}{8\pi\hbar} u(\alpha) R(\alpha) \right]^{1/2} \exp \left[-\frac{S_{B,1}^{(0)}}{2\hbar} \right], \quad (4.29)$$

where $u(\alpha)$, $R(\alpha)$, and $S_{B,1}^{(0)}(\alpha)$ are given in Eqs. (A10), (4.26), and (3.20b), respectively.

V. RESULTS AND DISCUSSION

Following the reasoning outlined in Sec. II, the decay rate Γ^+ is given by the formula

$$\Gamma^+ = \frac{\Delta^2}{2} \frac{1}{2i} \int_{\tau_s - i\infty}^{\tau_s + i\infty} d\tau_1 \exp[\sigma\tau_1 - P(\tau_1)], \quad (5.1)$$

in which the integral represents the contribution of the breathing mode. This term is the analytically continued integration over the length τ_1 of the bounce weighted by the exponential of the sum of the actions due to the asymmetry and due to the long-range intrabounce interaction. Using the explicit form (2.23) with $\omega_d = \omega_0$ for $P(\tau)$ the integral is found to yield the temperature dependent rate ($\beta \equiv 1/k_B T$)

$$\Gamma^+ = \frac{\Delta^2}{4\omega_0} \left[\frac{\beta\hbar\omega_0}{2\pi} \right]^{1-2\alpha_c} e^{\hbar\sigma\beta/2} \frac{|\Gamma(\alpha_c + i\beta\hbar\sigma/2)|^2}{\Gamma(2\alpha_c)}. \quad (5.2)$$

This formula has been derived first in Refs. 5 and 9, using a real time approach, and in Ref. 8 by means of the $\text{Im}F$ method. At zero temperature the rate Γ^+ simplifies for $\sigma > 0$ to the form

$$\Gamma^+ = \frac{\Delta^2}{2\omega_0} \frac{\pi}{\Gamma(2\alpha_c)} \left[\frac{\sigma}{\omega_0} \right]^{2\alpha_c - 1}, \quad (5.3)$$

while it vanishes for $\sigma < 0$. This result was previously obtained by Weiss *et al.*⁷ In the present paper we have calculated the dressed tunnel matrix element Δ , analytically, for the model potential (3.1).

We shall now compare the results contained in Eq. (4.29) with those derived on the basis of the truncation schemes proposed by Chakravarty and Kivelson³ and by Dorsey *et al.*⁴ These authors made estimates of the exponential part of the dressed tunnel matrix element $\Delta/2$. In the over-damped limit, $\alpha_c \gg 1$, they obtain

$$\frac{\Delta}{2} \sim \exp \left\{ -\alpha_c \left[\ln \left[\frac{8V_0}{\hbar\omega_0} \right] - \ln\alpha_c - c_\infty \right] \right\}, \quad (5.4)$$

where Dorsey *et al.*⁴ find $c_\infty = 1.24$, while Chakravarty and Kivelson give $c_\infty = 1.594$. Although our model potential differs from that considered by these groups of authors, the functional form (3.20), (3.22) and the numerical value of $c_\infty = +1.2606$, are in accord with the above results. This gives us confidence on the reasonableness of the results derived on the basis of the truncation schemes. These schemes, however, are unable to provide estimates of neither the magnitude nor the α dependence of the prefactor of the tunneling matrix element $\Delta/2$.

In the limit $\alpha_c \gg 1$ the integral in (5.1), which is due to the breathing mode, may be evaluated by the method of steepest descent. We then find for $T=0$ and $\sigma > 0$

$$\Gamma^+ = \frac{\Delta^2}{4\sigma} (4\pi\alpha_c)^{1/2} \exp[\sigma\tau_s - P(\tau_s)], \quad (5.5)$$

where τ_s is given in (3.13). This expression can be written in the standard form by means of the expression (4.29) for $\Delta/2$ and of (4.18) for the negative eigenvalue $\Lambda_0^{(B)}$

$$\begin{aligned} \Gamma &= A \exp[-S_{\text{ex}}(\tau_s)/\hbar], \\ A &= \omega_0 \left[\frac{M\omega_0 q_0^2 u(\alpha)}{4\pi\hbar} \right]^{1/2} \left[\frac{M\omega_0^2 R^2(\alpha)}{|\Lambda_0^{(B)}|} \right]^{1/2}, \end{aligned} \quad (5.6)$$

where the exponent is given in (3.23). The first square-root factor in the expression for A is due to the normalization of the zero mode of the bounce, while the second square-root factor is due to the fluctuation spectrum with the zero eigenvalue omitted. We find from (4.18), (4.28), and (A12) that for $\alpha \gg 1$ the prefactor A is given by

$$A = 2.042 \frac{8\sqrt{2}}{\pi^2} \left[\frac{V_0}{\hbar\omega_0} \right]^{1/2} \frac{V_0}{\hbar|\sigma|} \frac{\ln\alpha}{\sqrt{\alpha}} \omega_0. \quad (5.7)$$

The linear increase of the bounce action $S_{\text{ex}}[\tau_s]$ in (3.23) with α_c is in accord with the findings of Caldeira and Leggett.²⁴ The prefactor A of the decay rate varies as

$$A \sim \frac{\ln\alpha}{\sqrt{\alpha}}, \quad (5.8)$$

which decreases with increasing α . This result is somewhat surprising if one compares with the rapidly increasing $\alpha^{7/2}$ dependence of the prefactor found by Caldeira and Leggett for the decay in a potential with strong asym-

metry. The difference in the prefactors of the tunneling rates merits some discussion. In both physical situations the negative eigenvalue is independent of α for $\alpha \gg 1$. Also, the zero mode normalization factors show the same $\alpha^{-1/2}$ dependence in both cases. Hence, the difference is found in the contributions coming from the continuum of eigenvalues. Caldeira and Leggett²⁴ obtain the α^4 dependence from the asymptotic large α contribution of the integral in (4.8). For large α , one may replace the T matrix by the expression obtained from the first Born approximation. On assuming the validity of this formula down to $\Lambda = M\omega_0^2$ they obtain $R(\alpha) \sim \alpha^4$. In our case, we find that the corresponding expression is independent of α for $\alpha \rightarrow \infty$. In fact the leading $\ln\alpha/\alpha$ dependence found from the integration in (4.8) cancels with the leading $\alpha/\ln\alpha$ dependence of the coupling strength U . Hence, within the Born approximation, the two different physical situations lead to prefactors of the decay rate which differ by a factor α^4 in the limit of strong damping. In the exact calculation of our model the additional $\ln\alpha$ factor in Eq. (5.8) arises from the difference between the exact T matrix and the corresponding first Born approximation to the integrand in Eq. (4.8).

In the small α_c limit ($\alpha_c \ll 1$), we obtain the exponential part of the tunneling matrix element $\Delta/2$ as

$$\frac{\Delta}{2} \sim \exp \left[\frac{-2V_0}{\hbar\omega_0} - (C - \frac{1}{2})\alpha_c + \frac{3}{64} \frac{\hbar\omega_0}{V_0} \alpha_c^2 \right], \quad \alpha_c \ll 1, \quad (5.9)$$

where C is Euler's constant. This may be compared directly with the results of Dorsey *et al.*⁴ who find the coefficient of α_c to be given by the approximate expression

$$\left[\frac{3}{2} + C - \ln(2\pi) \right] \simeq 0.2392,$$

while Chakravarty and Kivelson³ find a value of $\simeq -0.2006$, which has the opposite sign. In our case, we find that the coefficient is given by the exact value

$$(C - \frac{1}{2}) \simeq 0.077,$$

which again lies intermediate between the two estimates. This suggests that although the estimates are of opposite sign, the discrepancy may be reconciled by the correct value being very close to zero.

Again, the truncation schemes are unable to produce estimates for the prefactor of $\Delta/2$. We find in our model, using Eqs. (4.3) and (4.27) that the $\alpha \rightarrow 0$ limit of the prefactor Ω of the tunneling matrix element $\Delta/2$ is given by the expression

$$\Omega = \omega_0 \left[\frac{2V_0}{\pi\hbar\omega_0} \right]^{1/2}, \quad \alpha_c \rightarrow 0. \quad (5.10)$$

Also, analytical expressions of the α dependent corrections to the formula (5.10) can be derived from the general expressions (4.3) and (4.26).

In summary, we have performed explicit calculations of the rate of incoherent tunneling in an asymmetric double well. Unlike most of the previous calculations by other

groups,¹⁻⁶ we have not truncated our system onto a two-state model. This allowed us to carry out explicit calculations for our potential. The expressions for both the exponent and the prefactor have been carried out exactly, within the dilute-bounce-gas approximation. Our expressions do not contain any undetermined functions. The exponential part of the rate has been found to be in good agreement with the estimates obtained with the truncation schemes,^{3,4} even though the models considered are not strictly equivalent. The prefactor of our rate contains contributions coming from the breathing mode, the time translational zero mode, and a continuum of modes. The contribution to the prefactor coming from the continuum of modes has not been evaluated previously, for incoherent quantum tunneling. We have calculated the prefactor exactly. We find that the prefactor only shows a weak variation with the dimensionless strength of the dissipation. This is in contrast with the prefactor of the rate associated with the tunneling out of a metastable state of a cubic potential.

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APPENDIX

In Secs. III and IV we have introduced the functions $K_j(\tau)$, $j=1,2,\pm$ and $\mathcal{J}_\pm(\tau)$. The functions $K_j(\tau)$ are defined by the integral representations

$$\begin{aligned} K_1(\tau) &= \omega_0^2 \frac{2}{\pi} \int_0^\infty d\omega \frac{\sin(2\omega\tau)}{\omega} \frac{1}{\omega^2 + \xi(\omega) + \omega_0^2}, \\ K_2(\tau) &= \omega_0 \frac{2}{\pi} \int_0^\infty d\omega \frac{\sin^2(\omega\tau)}{\omega^2} \frac{\xi(\omega)}{\omega^2 + \xi(\omega) + \omega_0^2}, \quad (A1) \\ K_\pm(\tau) &= \omega_0 \frac{1}{\pi} \int_0^\infty d\omega [1 \pm \cos(2\omega\tau)] \frac{1}{\omega^2 + \xi(\omega) + \omega_0^2}. \end{aligned}$$

In the case of Ohmic dissipation, where $\xi(\omega) = \gamma |\omega|$, these integrals can be expressed in terms of the auxiliary exponential integrals $f(z)$ and $g(z)$ defined on p. 232 of Ref. 31. In this case one obtains for $\tau > 0$

$$\begin{aligned} K_1(\tau) &= 1 + \frac{\omega_0}{\pi(\alpha^2 - 1)^{1/2}} \left[\frac{1}{\lambda_1} f(2\lambda_1\tau) - \frac{1}{\lambda_2} f(2\lambda_2\tau) \right], \\ K_\pm(\tau) &= \frac{1}{2} \left[s(\alpha) \pm \frac{1}{\pi(\alpha^2 - 1)^{1/2}} [g(2\lambda_2\tau) - g(2\lambda_1\tau)] \right], \quad (A2) \end{aligned}$$

where

$$\lambda_{1,2} = \omega_0 [\alpha \pm (\alpha^2 - 1)^{1/2}], \quad (A3)$$

and where $\alpha = \gamma/2\omega_0$. The function $s(\alpha)$ is given by

$$s(\alpha) = \begin{cases} \frac{2}{\pi(\alpha^2-1)^{1/2}} \ln[\alpha + (\alpha^2-1)^{1/2}], & \alpha \geq 1 \quad (\text{A4a}) \\ \frac{1}{(1-\alpha^2)^{1/2}} \left[1 - \frac{2}{\pi} \arcsin \alpha \right], & \alpha \leq 1, \quad (\text{A4b}) \end{cases}$$

and where $s(1) = 2/\pi$

The function $K_2(\tau)$, $\tau > \sigma$, must be evaluated with care, since it contains mutually compensating divergences. The explicit form emerges as

$$K_2(\tau) = \frac{2\alpha}{\pi} \left\{ C + \ln(2\omega_0\tau) + \frac{\omega_0}{2(\alpha^2-1)^{1/2}} \left[\frac{1}{\lambda_2} \ln \left[\frac{\lambda_2}{\omega_0} \right] - \frac{1}{\lambda_1} \ln \left[\frac{\lambda_1}{\omega_0} \right] \right] + \frac{\omega_0}{2(\alpha^2-1)^{1/2}} \left[\frac{1}{\lambda_2} g(2\lambda_2\tau) - \frac{1}{\lambda_1} g(2\lambda_1\tau) \right] \right\}, \quad (\text{A5})$$

where C is Euler's constant.

These functions may be evaluated asymptotically in the region

$$\lambda_1\tau \gg 1, \quad \lambda_2\tau \gg 1, \quad (\text{A6a})$$

which for small α is equivalent to

$$\omega_0\tau \gg 1, \quad (\text{A6b})$$

while for $\alpha \gg 1$

$$\frac{\omega_0\tau}{\alpha} \gg 1. \quad (\text{A6c})$$

We then find

$$K_1(\tau) = 1 - \frac{2\alpha}{\pi} \frac{1}{\omega_0\tau} + O(\tau^{-3}),$$

$$K_{\pm} = \frac{1}{2} \left[s(\alpha) \pm \frac{\alpha}{\pi} \frac{1}{(\omega_0\tau)^2} + O(\tau^{-4}) \right],$$

$$K_2(\tau) = \frac{2\alpha}{\pi} \left\{ C + \ln(2\omega_0\tau) + \frac{\omega_0}{2(\alpha^2-1)^{1/2}} \left[\frac{1}{\lambda_2} \ln \left[\frac{\lambda_2}{\omega_0} \right] - \frac{1}{\lambda_1} \ln \left[\frac{\lambda_1}{\omega_0} \right] \right] + \frac{1}{\lambda_2} \frac{1}{(2\lambda_2\tau)^2} - \frac{1}{\lambda_1} \frac{1}{(2\lambda_1\tau)^2} \right\} + O(\tau^{-4}). \quad (\text{A7})$$

Next, we define the functions $\mathcal{F}_{\pm}(\tau)$ occurring in the normalization of the modes $\varphi_0^{(B)}(\tau)$ and $\varphi_1^{(B)}(\tau)$,

$$\mathcal{F}_{\pm}(\tau) = \frac{4}{\pi} \omega_0^3 \int_0^{\infty} d\omega \frac{[1 \pm \cos(\omega\tau)]}{[\omega^2 + \omega_0^2 + \xi(\omega)]^2}. \quad (\text{A8})$$

For Ohmic dissipation these functions are related to the functions $K_{\pm}(\tau)$ defined above by

$$\mathcal{F}_{\pm}(\tau) = 4\omega_0^2 \frac{\partial}{\partial \lambda_1} \frac{\partial}{\partial \lambda_2} K_{\pm}(\tau).$$

The resulting expressions can again be expressed in terms of the auxiliary exponential integrals $g(z)$ and $f(z)$. In the asymptotic region we find

$$\mathcal{F}_{\pm}(\tau) = u(\alpha) \pm \frac{16\alpha}{\pi} \left[\frac{1}{\omega_0\tau} \right]^2 + O(\tau^{-4}), \quad (\text{A9})$$

where the function $u(\alpha)$ is defined by

$$u(\alpha) = \frac{1}{\alpha^2-1} \left[\frac{2}{\pi} \alpha - s(\alpha) \right], \quad (\text{A10})$$

and where $s(\alpha)$ is given in (A4). For weak damping $\alpha \ll 1$ we find

$$u(\alpha) = 1 - \frac{4}{\pi} \alpha + O(\alpha^2), \quad (\text{A11})$$

and for strong damping $\alpha \gg 1$

$$u(\alpha) = \frac{2}{\pi} \frac{1}{\alpha} \left[1 - \frac{\ln(2\alpha)}{\alpha^2} + O(\alpha^{-2}) \right]. \quad (\text{A12})$$

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