

Macroscopic Quantum Tunneling at Finite Temperatures^a

PETER HANGGI

*Department of Physics
Polytechnic Institute of New York
Brooklyn, New York 11201*

INTRODUCTION

There are a great variety of phenomena in physical, chemical, and biological sciences that are caused by transitions between locally stable states. In the absence of thermal and quantal fluctuations, no such transitions would occur; that is, the states would remain stable. Over the last few years, the common theme underlying the description of escape processes has been based on Brownian motion theory. In adapting this theme, the motion of the principal degrees of freedom is treated explicitly, while the interactions with the other degrees of freedom, including those of the environment (heat baths) coupled to the system of interest, are represented by frictional forces and random noise. The noise represents the key input, thus allowing the system to get away from preferred states of local stability. At high temperatures, thermal activation is the dominant process wherein a particle hops over the intervening potential barrier. This process has been studied in its various complexities in great detail over the last two decades.^{1,2} When the temperature is lowered, thermally activated hopping processes become rarer and the effect of quantum tunneling becomes increasingly important.

Mainly inspired by ideas of Anthony Leggett,^{3,4} there has been renewed interest in the quantum dynamics of a system where dissipation is important. In particular, there is the problem of low temperature tunneling and coherence of macroscopic quantum variables. These processes are necessarily also subject to dissipative forces. Ideal experimental systems where the predicted phenomena might be observable are the decay of the zero-voltage state in a current biased Josephson junction, or the fluxoid quantum transitions in a single junction superconducting quantum interference device (SQUID) ring. In the first case, the macroscopic quantum variable is given by the phase difference across the junction, while in the latter case, the appropriate macroscopic variable is the magnetic flux trapped through the ring. Encouraged by a set of recent experiments⁵⁻⁷ that are in qualitative agreement with theory, this field has seen many rapid new developments.^{2,8,9} Caldeira and Leggett³ have shown that the tunneling probability at zero temperature is strongly affected by the dissipation that results in a strong suppression of the decay rate. Furthermore, at finite temperatures, Grabert, Weiss, and Hanggi¹⁰ found a drastic change of the temperature dependence of the tunneling probability in the presence of dissipation. Apart from the phenomenon of macroscopic quantum tunneling, other macroscopic quantum effects have recently

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been predicted. In particular, they are:

- (i) the phenomenon of coherent oscillations in a symmetric^{8,9,11} or in a weakly asymmetric double well^{12,13} in the presence of Ohmic-like dissipation;
- (ii) macroscopic energy quantization;¹⁴
- (iii) Bloch oscillations in Josephson junctions that are driven by a weak external current.¹⁵

The decay of a metastable quantum state is usually referred to as "macroscopic quantum tunneling" (MQT), whereas the phenomenon of damped, coherent oscillations of a macroscopic quantum variable between two almost degenerate, distinct macroscopic states is known as "macroscopic quantum coherence" (MQC).¹¹ Interestingly enough, the very recent, appealing experiments by Washburn *et al.*^{16,17} on MQT in the regime of moderate Ohmic-like friction, and by Schwartz *et al.*¹⁸ in the strongly overdamped friction regime, have confirmed quantitatively many of the predicted universal temperature effects^{2,9,10} of Ohmic-like dissipation. As of yet, MQC experiments^{7,19} have not been carried out.

In the following, we restrict the discussion to dissipative MQT only, elaborating on the historic background, the method, the results, and a discussion of the regime of validity.

HISTORIC BACKGROUND AND STATEMENT OF THE PROBLEM

The quantum description of metastable and unstable states has been a subject of many investigations since the early days of quantum mechanics. As is well known, the description of such states gives rise to several conceptual problems that arise from the difficulty of finding a satisfactory characterization of these states. There are several methods available in the literature²⁰ that characterize the decay of a metastable state at zero temperature. Some of the more familiar ones are:

- (a) The axiomatic S-matrix theory,^{20,21} wherein one associates decay rates in a one-to-one correspondence with poles of the S-matrix close to the real axis on the unphysical sheet of the energy Riemann surface, provided that the S-matrix can be analytically continued there.
- (b) A time-dependent wave function approach, whereby one considers the outgoing scattering wave near a resonance energy.^{20,22} In this case, there occurs a typical time delay, $t_D = 2/\Gamma$, in the arrival of the scattered wave of the order of the inverse decay rate, Γ , with respect to the case in which no resonance occurs.
- (c) A dynamical semigroup approach for the evolution of the density operator.²³

The approaches in (a) and (b) are not readily extended to finite temperatures and to situations where the interactions with the environment become important. For the following, we should also remind ourselves that a pure exponential decay at all times can only occur if a rescattering from the decay products (backscattering) were to be absent. However, the rescattering phenomenon cannot be forbidden unless one chooses a Hamiltonian that is not bounded from below. Khalfin²⁴ has pointed out, by use of a fundamental theorem of Paley and Wiener,²⁵ that the quantum nondecay probability,

$P(t)$, cannot be purely exponential for very large times if the minimum of the energy spectrum of the Hamiltonian is bounded from below at $E_{\min} \neq -\infty$. Moreover, the quantum nondecay probability then also possesses a vanishing derivative at the origin of time evolution; that is, $P(t)$ is also not of exponential form for very short times. Throughout the rest of the paper, therefore, we will focus our attention only on the decay law at intermediate times for which the decay law has approximately exponential form. In practice, this intermediate time regime is very large;²⁰ it usually extends over a time scale at which 99% of the reduction in $P(t)$ has occurred already.

Over the last two decades, probably the most developed theory to describe dissipative quantum mechanics²⁶ at finite temperatures has been the semigroup approach.²³ This type of method has been very popular in describing damping phenomena in nonlinear optics²⁷⁻²⁹ and in spin relaxation theory.²⁹ However, these dissipative semigroup methods treat the coupling to the environment perturbatively. This restricts the treatment only to the weak damping regime, where the largest damping coefficient, γ , typically obeys²⁹

$$\gamma \ll \omega_0, \quad \hbar\gamma \ll kT. \quad (1)$$

Here, ω_0 is the smallest frequency typical for reversible motion. In a tunneling system, ω_0 may differ from zero just by the tunnel splitting. Thus, the first inequality is violated already for very weak damping. Furthermore, macroscopic tunneling phenomena occur at extreme low temperatures; that is, the second inequality is then also violated for an appreciable amount of dissipation. Hence, for tunneling systems, a more accurate description of dissipation is needed.

THE FUNCTIONAL INTEGRAL APPROACH

As is well known, tunneling problems are advantageously treated in terms of complex-time path integrals.^{2,3,9} A detailed description of all aspects of this method is certainly beyond the scope of this article. Here, therefore, I will confine myself to a brief outline only, wherein I will present the main ingredients of the method. First, let us consider the partition function,

$$Z = \text{tr} \exp(-\beta H), \quad \beta = 1/(kT). \quad (2)$$

Following Feynman,³⁰ this quantity can be expressed (without having to refer to any dubious analytic continuation tricks) in the form of a (Euclidian) functional path integral,

$$Z = \int \mathcal{D}q(\tau) \exp\{- (S_E[q(\tau)]/\hbar)\}. \quad (3)$$

The integral in equation 3 runs over all paths that are periodic with period $\theta = \hbar\beta$. Each path is weighted by the Euclidian action, S_E . For our applications, we also must account for the dissipation being induced by the coupling of the tunneling coordinate to the heat bath. In doing so, we start out from the functional integral expression in full phase-space of particle plus environment. Furthermore, we assume that the environmental degrees of freedom couple bilinearly to the tunneling coordinate. If we present the environmental degrees (bath modes) by a set of harmonic oscillator modes, one

succeeds in integrating out the bath modes exactly.^{3,30} This procedure leaves one with an effective action that models the influence of dissipation by a nonlocal term. For Ohmic dissipation,

$$\ddot{q} = -\frac{1}{M} \frac{\partial V}{\partial q} - \gamma \dot{q}, \quad (4)$$

so the result obtained for the effective (Euclidian) action is^{9,10}

$$S_E[q] = \int_{-\theta/2}^{\theta/2} d\tau [\frac{1}{2} M \dot{q}^2 + V(q)] + \frac{1}{2} \int_{-\theta/2}^{\theta/2} d\tau \int_{-\theta/2}^{\theta/2} d\tau' k(\tau - \tau') q(\tau) q(\tau'). \quad (5)$$

The first term describes the reversible motion of the particle in the absence of an environmental coupling. The second nonlocal term, given here in the form used by Grabert *et al.*,¹⁰ describes the influence of dissipation. For the Ohmic dissipation in equation 4, it has the explicit form,^{9,10}

$$k(\tau) = \frac{M}{\theta} \sum_{n=-\infty}^{n=+\infty} |\nu_n| \gamma \exp(i\nu_n \tau), \quad \theta = \hbar\beta, \quad (6a)$$

with

$$\int_{-\theta/2}^{\theta/2} k(\tau) d\tau = 0, \quad (6b)$$

and $\nu_n = n2\pi/\theta$ being the Matsubara frequency. In addition, the dissipative, nonlocal part can alternatively be recast in the form used by Bray and Moore,¹¹

$$-\frac{1}{4} \int_{-\theta/2}^{\theta/2} d\tau \int_{-\theta/2}^{\theta/2} d\tau' k(\tau - \tau') [q(\tau) - q(\tau')]^2, \quad (6c)$$

which reveals explicitly the translational invariance of the dissipative part of the effective action.

Instead of the presented Euclidian (imaginary-time) formulation, a real-time formulation, being necessary for the problem of MQC, can also be used. This objective is advantageously treated by use of Feynman-Vernon theory.^{31,32} Let $P_o(q)$ be the probability density of the tunneling particle in configuration space, q , at initial time, $t = 0$. Then, the probability, $P_t(q)$, at time, t , may be recast in the form of a double path integral,^{12,32}

$$P_t(q) = \int \mathcal{D}q \int \mathcal{D}q' \exp \{i(S_o[q] - S_o[q'])/\hbar\} \cdot \exp(i\phi[q, q']/\hbar) \cdot P_o(q_o), \quad (7a)$$

where the integral is over all paths of $q(s)$, $q'(s)$, and $0 \leq s \leq t$, with $q(0) = q'(0) = q_o$; $q(t) = q'(t) = q$, and q_o being integrated over. S_o denotes the unperturbed (Minkowskian) action,

$$S_o[q] = \int_0^t ds \{1/2 M \dot{q}^2(s) - V[q(s)]\}. \quad (7b)$$

For Ohmic dissipation, the influence functional, $\phi[q, q']$, is given by^{12,32}

$$\begin{aligned} \phi[q, q'] = & \int_0^t ds \int_0^s ds' [\dot{q}(s) - \dot{q}'(s)] \\ & \cdot [Q(s - s') \dot{q}(s') - Q^*(s - s') \dot{q}'(s')], \quad (7c) \end{aligned}$$

where

$$Q(s) = \frac{M\gamma}{\pi} \ln \{ (\hbar\beta \omega_0/\pi) \sinh (s\pi/\hbar\beta) \} + 1/2 iM\gamma, \quad (7d)$$

and $\omega_0^2 = V''(q_{\min})/M$ denotes the angular frequency at the well bottom. Both the Euclidian-time formulation (equations 3 and 5) and the real-time representation (equation 7) are suitable starting points to discuss tunneling phenomena in the presence of dissipative interactions.

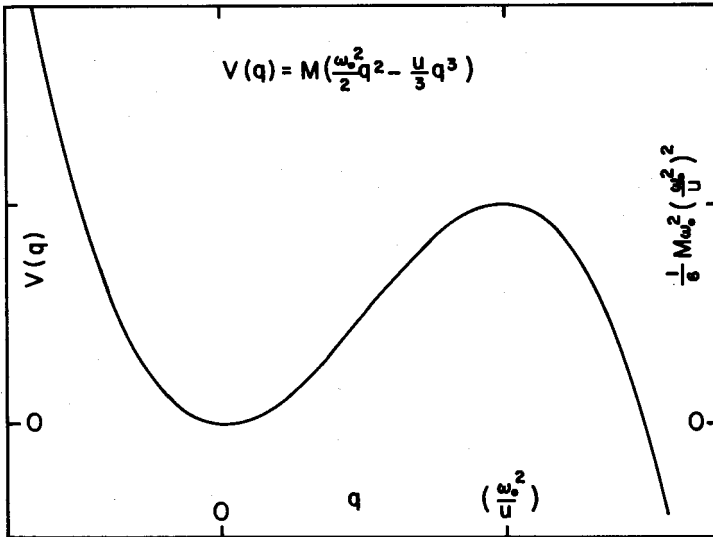


FIGURE 1. The metastable potential field, $V(q) = M [1/2\omega_0^2 q^2 - 1/3uq^3]$, used in the text. The top of the barrier is located at $q_b = \omega_0^2/u$.

THE TUNNELING RATE

Now we are prepared enough to discuss the MQT decay in a metastable potential field, $V(q)$, of the form depicted in FIGURE 1. Initially, the particle is located near $q = 0$. The free energy, F , of the particle is then given by (see equation 3)

$$F = -kT \ln Z = -kT \ln \left\{ \int \mathcal{D}q \exp (-S_E[q]/\hbar) \right\}, \quad (8)$$

with S_E given as in equations 5 and 6. The state near $q = 0$ is metastable if its lifetime, $\tau_0 = \Gamma^{-1}$, is long compared to all other characteristic time scales that describe the relaxation towards the locally stable state at $q = 0$. Keeping this situation in mind, it turns out that the functional integral in equation 8 is not real, but possesses an exponentially small imaginary part that is proportional to the decay rate, Γ . This fact should, of course, not come as too big of a surprise. After all, we are attempting to compute a decay rate that is not part of the spectrum of a Hamiltonian that is bounded

from below. This same difficulty has already been seen in Langer's picture modeling classical nucleation.³³ For the problem of quantum decay at zero temperature and vanishing dissipation, Callan and Coleman³⁴ beautifully popularized Langer's technique. They explained that the free energy can still be defined if one uses an analytic continuation from a stable to an unstable situation. An evaluation of the integral in equation 8 can be obtained by summing the contributions of the paths that make the Euclidian action (equation 5) stationary or almost stationary. As is evident from equation 5, the Euclidian action is stationary for those paths that are solutions of the classical equation of motion in an inverted potential, $V(q) \rightarrow -V(q)$; that is,

$$M\ddot{q}_B = \frac{\partial V}{\partial q_B} + \int_{-\theta/2}^{\theta/2} d\tau' k(\tau - \tau') q_B(\tau') \quad (9)$$

with $q_B(\tau)$ obeying the periodic boundary condition of

$$q_B(\tau - 1/2\theta) = q_B(\tau + 1/2\theta). \quad (10)$$

Because of equation 6b, we also observe that equation 9 possesses two trivial solutions: $q_1(\tau) = 0$, where the particle just sits on top of the inverted potential, $-V(q)$, and $q_2(\tau) \equiv q_b = \omega_0^2/u$ (see FIGURE 1), where the particle is located at the minimum of the well of $-V(q)$. Equation 9 possesses a nontrivial solution at sufficiently low temperatures, T , below a certain crossover temperature, T_o .^{10,35,36}

$$T_o = (\hbar/2\pi k) [(\omega_b^2 + 1/4\gamma^2)^{1/2} - 1/2\gamma], \quad \omega_b^2 = -V''(q_b)/M. \quad (11)$$

At temperatures, $T < T_o$, the solution, $q_B(\tau)$ (see equation 9), describes an oscillating motion in the classically forbidden regime. Coleman has coined the name "bounce" for this particular tunneling trajectory. In FIGURE 2, we depict this bounce solution for the potential field in FIGURE 1 at various temperatures. Below $T < T_o$, the trivial solution, $q_2(\tau) = q_b$, can be disregarded. FIGURE 3 shows the "entrance" and the "exit" points of the bounce solution. The difference in energy between these two reference points may then be identified with the energy loss in quantum tunneling.³⁷ At zero temperature, this energy loss is always negative, and it has the characteristic feature that it saturates for increasing strength of dissipation.³⁷ At finite temperatures, however, the particle may lose or gain energy in tunneling across the potential barrier.³⁸

The detailed analysis shows that the solutions of $q_B(\tau)$, $T < T_o$ (or $q = q_b$ for $T > T_o$), are not minima of the action S_E , but represent a saddle-point solution. This simply means that there is one fluctuation mode in function space with respect to which the bounce is a maximum of the action. This characteristic fluctuation mode thus has a negative eigenvalue. This obviously plagues the evaluation of the partition function. What is needed here is an analytical continuation, mentioned above, where the integral of the unstable (negative eigenvalue) mode is distorted in the complex plane so that it passes through the saddle point and then into the complex plane.^{33,34} If we observe that the canonical operator, $\exp(-\beta H)$, is the evolution operator for imaginary times, $\tau = -i\hbar\beta$, we find that with a decay rate of Γ , that is,

$$\tau H \rightarrow \tau(H - 1/2i\hbar\Gamma), \quad (12)$$

the exponentially small complex part of the free energy obeys the relation,^{2,9,35-39}

$$\Gamma = -(2/\hbar) \text{Im } F. \quad (13)$$

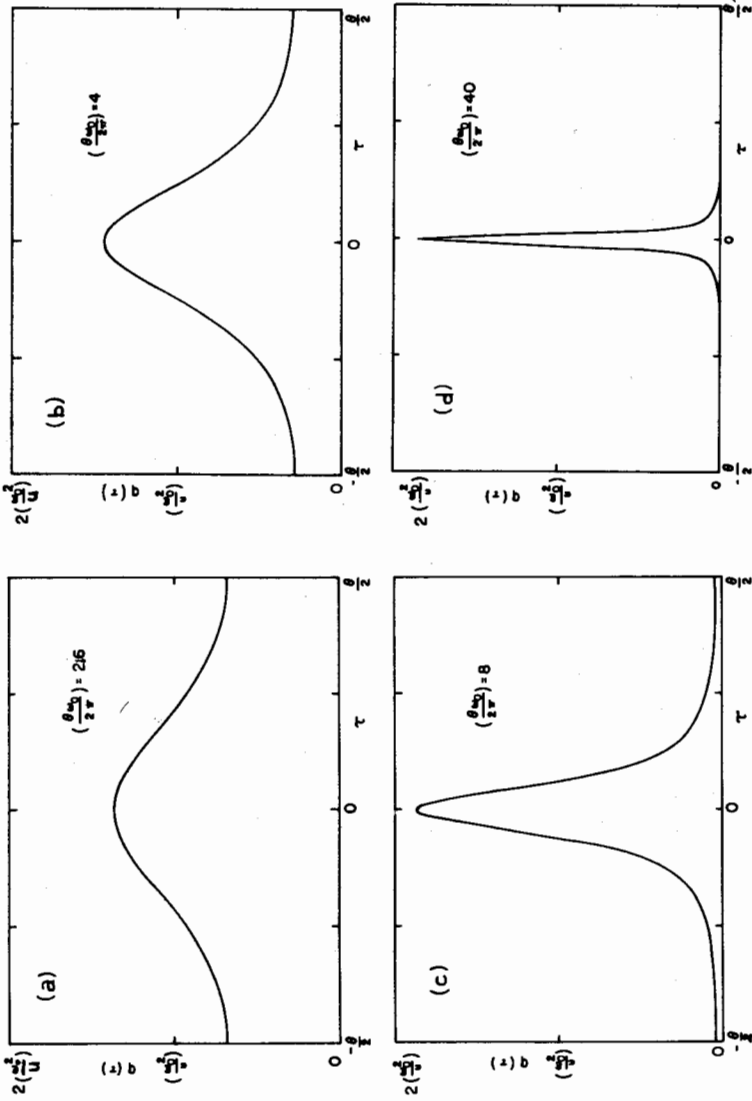


FIGURE 2. The bounce trajectories for the potential in FIGURE 1 at moderate friction strength, $\gamma/\omega_0 = 2$, for a sequence of decreasing temperatures, $\theta = \hbar\beta$.

For temperatures above T_o , a detailed evaluation of equations 8 and 13 then gives

$$\Gamma = (kT_o/\hbar) \left\{ \frac{\text{Det}(\delta^2 S_E/\delta q^2)q(\tau) - 0}{|\text{Det}(\delta^2 S_E/\delta q^2)q(\tau) - q_b|} \right\}^{1/2} \exp(-\beta E_b), \quad T > T_o, \quad (14)$$

where E_b denotes the barrier height. For strict Ohmic dissipation (see equation 4), this explicitly yields^{35,36,40,41}

$$\Gamma = (kT_o/\hbar) \frac{\omega_0}{\omega_b} \left(\prod_{n=1}^{\infty} \frac{n^2 \nu^2 + \omega_0^2 + n\nu\gamma}{n^2 \nu^2 - \omega_b^2 + n\nu\gamma} \right) \exp(-\beta E_b), \quad (15)$$

where $\nu = 2\pi/\theta$, $\omega_0^2 = V''(q=0)/M$, and $\omega_b^2 = -V''(q_b)/M$. The above result can also

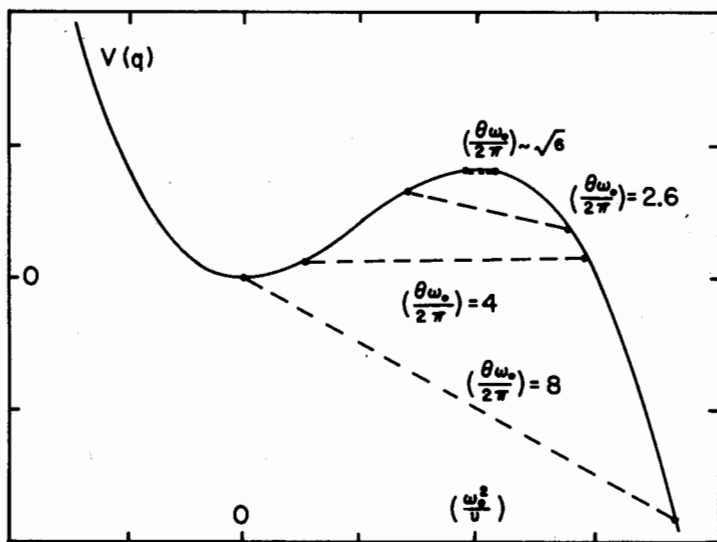


FIGURE 3. The variation of the extrema of the bounce trajectories as the temperature is decreased. At the crossover temperature, T_o , the bounce remains at the top of the potential barrier at $q_b(\tau) = q_b$.³⁸

be generalized to the case of memory friction, $\gamma(t)$;⁴⁰ that is,

$$\ddot{q} = -\frac{1}{M} \frac{\partial V}{\partial q} - \int_0^t \gamma(t-s) \dot{q}(s) ds. \quad (16)$$

Then, in equation 15, we only have to substitute γ by $\hat{\gamma}(n\nu)$, where $\hat{\gamma}(z)$ denotes the Laplace transform of the memory friction, $\gamma(t)$. For memory damping (equation 16), the crossover temperature, T_o , will also be memory-renormalized to give⁴⁰

$$T_o = \hbar\mu/(2\pi k) \quad (17)$$

with μ being the largest positive root of

$$\mu^2 + \mu\hat{\gamma}(\mu) = \omega_b^2. \quad (18)$$

Combining equations 16 and 17 with equation 15, we can recast the result for the decay rate in the form of

$$\Gamma = \left\{ (\mu/\omega_b) \frac{\omega_0}{2\pi} \exp(-\beta E_b) \right\} Q, \quad T > T_o. \quad (19)$$

The term in the braces just equals the classical, dissipation, and memory renormalized thermal activation rate.⁴² The factor Q accounts for the quantum effects at $T > T_o$, namely,

$$Q = \prod_{n=1}^{\infty} \frac{n^2\nu^2 + \omega_0^2 + n\nu\hat{\gamma}(n\nu)}{n^2\nu^2 - \omega_b^2 + n\nu\hat{\gamma}(n\nu)} \geq 1, \quad (20)$$

and approaches unity for $T \gg T_o$. This quantum correction can be quite large, even at temperatures of the order of a few T_o . Thus, these deviations from the classical hopping rate are essential in a precise analysis of parameters in MQT experiments.^{16-18,43} There exists, then, a very useful, simple working approximation to the quantum enhancement factor Q , which reads⁴⁰

$$Q \approx \exp \left[\frac{\hbar^2 (\omega_0^2 + \omega_b^2)}{24 (kT)^2} + O(T^{-4}) \right]. \quad (21)$$

This approximation is most accurate for weak-to-moderate zero-frequency friction, denoted by γ_0 , where

$$\gamma_0 = \hat{\gamma}(z=0) \approx O(\omega_b). \quad (22)$$

It also becomes even more accurate for a dissipative mechanism with a large memory friction relaxation time.⁴⁰ The effect of quantum tunneling thus results essentially in a T -dependent renormalization of the barrier (Arrhenius) factor towards smaller values. In FIGURE 4, we depict this quantum correction Q (see equation 20) together with the working approximation in equation 21. It should also be noted here that the approximation of the order T^{-2} does not depend on the detailed dissipative mechanism. In contrast, the crossover temperature, T_o , depends via equation 18 on the amount and form of dissipation: For fixed zero-frequency dissipation, γ_0 , the crossover temperature is monotonically increasing towards its undamped value, $\mu = \omega_b$, with increasing memory friction relaxation time.⁴⁰

At temperatures below T_o , though, the relevant contribution to the decay rate is made up by the bounce. This bounce trajectory, however, is not uniquely defined in the sense that a translation, $q_B(\tau) \rightarrow q_B(\tau + b)$, also generates a solution that leaves the Euclidian action invariant. This invariance of the action S_E (equation 5) is revealed by an eigenmode, $y_1(\tau) \propto \dot{q}_B(\tau)$, with zero eigenvalue, $\lambda_1 = 0$. This means that an infinitesimal translation ϵ in $q_B(\tau)$ does not change the action: The variation of

$$y(\tau) = q_B(\tau + \epsilon) - q_B(\tau) = \dot{q}_B(\tau)\epsilon$$

gives $\delta S_E = 0$. The best medicine to take in order to avoid the difficulties generated by

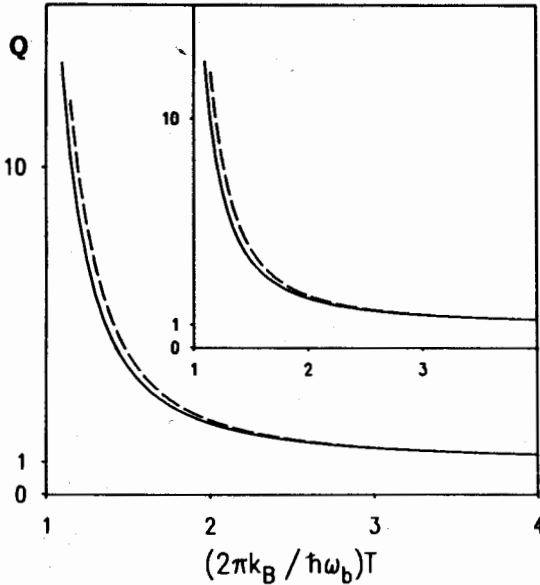


FIGURE 4. The approximation (dashed line) of equation 21 for the quantum correction factor Q compared with the exact expression of equation 20 (solid line) for a memory damping $\gamma(t) = \kappa\omega_b J_1(\kappa\omega_b t/r)/t$, with $\omega_b = \omega_0$, $\kappa = 0.5$, and $r = 0.25$. The inset shows the same for an exponential memory damping $\gamma(t) = \kappa\omega_b/\tau_c \exp(-t/\tau_c)$, with $\omega_b = \omega_0$, $\kappa = 0.5$, and $\omega_b \cdot \tau_c = 0.5$.⁴⁰

this zero-mode is to perform a change of coordinates and to integrate directly over the translation variable b ,³⁴ rather than over the zero-mode $y_1(\tau)$. Following the recipe of Faddeev and Popov⁴⁴ (gauge fixing condition; see also references 35 and 38), one finds that this procedure induces a zero-mode normalization factor, A , where

$$A = \left\{ \frac{M}{2\pi\hbar} \int_{-0/2}^{0/2} \dot{q}_B^2(\tau) d\tau \right\}^{1/2}. \tag{23}$$

Thus, the final result for the decay rate at $T < T_o$ is given by^{2,9,10,35,38}

$$\Gamma = A \left\{ \frac{\text{Det}(\delta^2 S_E / \delta q^2) q(\tau) = 0}{|\text{Det}'(\delta^2 S_E / \delta q^2) q(\tau) = q_B(\tau)|} \right\}^{1/2} \exp[-S_B(\theta, \dot{\gamma})/\hbar], \quad T < T_o. \tag{24}$$

Here, $S_B(\theta, \dot{\gamma})$ is the bounce action, $S_B(\theta, \dot{\gamma}) = S_E[q_B(\tau)]$, and the prime indicates that the eigenvalue zero is to be omitted. At temperature, $T = T_o$, the bounce action, S_B/\hbar , matches smoothly with the Arrhenius factor, E_b/kT_o .^{10,38} An analytical evaluation of equation 24 is possible only for the cubic potential shown in FIGURE 1 at weak^{3,38,39} and very strong Ohmic damping^{3,35,38} (see equation 4), and at one particular moderate friction value.³⁸ In practice, one must therefore resort to a numerical evaluation (see reference 45 for $T = 0$ and reference 46 for $0 \leq T \leq T_o$).

Just as in the case of $T > T_o$, where the prefactor is increasing with increasing memory relaxation time,⁴⁰ and with γ_0 held fixed, we find that the decay rate is exponentially enhanced with increasing memory friction relaxation time (decrease of S_B for fixed dissipation strength, γ_0 , and fixed dimensionless temperature, θ/θ_o).⁴⁷

The low temperature behavior of equation 24, however, exhibits a universal behavior. Grabert, Weiss, and Hanggi¹⁰ have shown that the temperature enhance-

ment follows a characteristic power law,¹⁰

$$S_B(T, \hat{\gamma}) = S_B(T = 0, \hat{\gamma}) - \frac{\pi}{6} \gamma_o M q_o^2 (kT\tau_B/\hbar)^2, \tag{25a}$$

where in terms of the tunneling distance, q_o , with $V(q = 0) = 0 = V(q_o)$, the bounce length, τ_B , is defined by

$$q_o \tau_B = \int_{-\infty}^{\infty} q_B(T = 0, \hat{\gamma}; \tau) d\tau. \tag{25b}$$

The law, $\ln[\Gamma/\Gamma(T = 0)] \propto T^2$, holds for all systems with Ohmic-like damping, namely, where $\hat{\gamma}(z = 0) = \gamma_o > 0$. The factor of proportionality depends via equation 25b on potential form and dissipation strength only. For example, for a weakly asymmetric double well potential with bias $\hbar\sigma$, $\sigma < 0$ (see FIGURE 5), the bounce length, τ_B , is estimated to be³⁷

$$\tau_B = M\gamma_o q_o^2 / (\pi\hbar |\sigma|) \equiv 2\alpha_c / |\sigma|. \tag{26}$$

In this case, the zero-temperature incoherent tunneling rate, Γ_o , is a nonanalytic function of the bias. It explicitly reads³⁷

$$\Gamma_o = \frac{\pi \Delta^2}{2 \omega_o} \frac{1}{\Gamma(2\alpha_c)} \left(\frac{|\sigma|}{\omega_o} \right)^{2\alpha_c - 1}, \quad \alpha_c > 1/2, \tag{27a}$$

where Δ^2 denotes the friction renormalized tunneling matrix element. From equation 25a, we then find for the low temperature enhancement,

$$\ln [\Gamma(T)/\Gamma_o] = \frac{4 \pi^2 \omega_o^2}{3|\sigma|^2} \alpha_c^3 \left(\frac{kT}{\hbar\omega_o} \right)^2. \tag{27b}$$

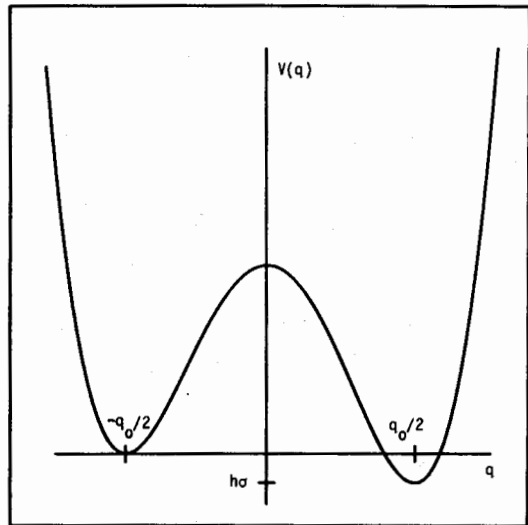


FIGURE 5. A slightly asymmetric double well in which incoherent Ohmic tunneling occurs with a rate given by equations 27 and 28.

For moderate-to-large friction, α_c , this result coincides with the leading low temperature behavior of a more elaborate treatment:^{12,13}

$$\Gamma(T) = \frac{1}{2} \frac{\Delta^2}{\omega_o} \left(\frac{\hbar\beta\omega_o}{2\pi} \right)^{1-2\alpha_c} \cosh(\hbar\beta\sigma/2) \frac{|\Gamma(\alpha_c + i\hbar\beta\sigma/2\pi)|^2}{\Gamma(2\alpha_c)}. \quad (28)$$

The detailed behavior of the rate close to crossover, $T \approx T_o$, is again more complicated because of the occurrence of a second quasi zero-mode.³⁶ As can be seen in FIGURE 2, the bounce solution, $q_B(\tau)$, approaches the trivial solution, $q_B(\tau) = q_b$, more closely as $T \uparrow T_o$. Thus, any linear combination of the two solutions is an almost stationary solution of the Euclidian action. Each one of these two quasi-stationary solutions separately induces a quasi zero-mode (an exact zero-mode and a quasi zero-mode^{36,38}). This problem is best dealt with by treating the two dangerous modes in the effective action, S_E , up to cubic and quartic order.^{35,36,38} Moreover, Grabert and Weiss³⁶ have shown that near $T \approx T_o$, there exists a frequency scale Λ and a temperature scale x_o (which depend on the particular system under consideration) such that in the region of $|T - T_o| \leq x_o$, the rate exhibits a universal scaling behavior; that is,^{9,36}

$$\Gamma/\Lambda = \text{Erfc}(\chi) \exp(\chi^2), \quad \chi = (T - T_o)/x_o, \quad (29)$$

where $\text{Erfc}(\chi)$ is the integral, $2\pi^{-1/2} \int_{-\infty}^{\chi} dt \exp(-t^2)$.

DISCUSSION

In this final section, we comment on the regime of validity of the dissipative MQT rates derived in equation 19 for $T > T_o$ and in equation 24 for $T < T_o$. As mentioned previously, the rate expression for temperatures above crossover (see equation 19) approaches the classical activation rate,^{1,2,42} which is valid for moderate-to-large friction strength; that is,²

$$\hat{\gamma}(\mu) \geq \omega_b, \quad T > T_o. \quad (30)$$

For high barrier factors, $\beta E_b \gg 1$, the regime of friction values for which the thermal equilibrium population is maintained in the initial well (yielding the formula for the decay rate in equation 14) extends to even lower friction where the Kramers theory^{1,2,42} approaches the result of standard transition-state-theory;² that is, the regime extends to weak-to-moderate-to-large friction, obeying

$$\hat{\gamma}(\mu) \geq kT\omega_b/E_b, \quad T > T_o. \quad (31)$$

In other words, with a high potential barrier, the time scale for escape is so large that the thermalization in the initial well then occurs even for weak damping (equation 31); that is, it occurs on such a sufficiently slow time scale that deviations from the thermal equilibrium distribution inside the well can safely be neglected. For even weaker damping, however, deviations from thermal equilibrium start to play a role. For such small friction values, that is, for^{2,48}

$$\int_0^{\infty} \gamma(t) \cos(\omega_o t/2\pi) dt < kT/J(E_b) \approx kT\omega_b/E_b \quad (32)$$

with $J(E_b)$ denoting the classical (Minkowskian) action at energy E_b^- , the rate dominating mechanism is energy diffusion.² For extreme weak friction, $\hat{\gamma}(\mu) \ll kT\omega_b/E_b$, the classical activation rate vanishes proportional to the dissipation strength.^{1,2,48,49} Clearly, the rate never vanishes completely in practice; it is bounded from below by the tunneling rate at low temperatures. The quantum corrections for $T > T_o$ for weak-to-moderate-to-large friction, as specified by equations 30 and 31, are given by the factor Q in equations 20 and 21. For extreme weak damping (equation 32), there occur above crossover, $T > T_o$, (apart from the ever-present quantum correction in equations 20 and 21) additional small quantum corrections^b to the weak damping classical hopping rate that are of the type discussed recently by Melnikov⁵⁰ and Larkin and Ovchinnikov.⁵¹ For this small regime of very weak friction, the precise form of these corrections (which originate from the quantum effects on the high temperature deviations from the thermal equilibrium population inside the well) are not known as of the present time; it is only known that the corrections derived in references 50 and 51 do not approach the correct classical limiting weak friction results obtained recently by Risken and Voigtlaender.⁵²

For temperatures below crossover, $T < T_o$, the quantum tunneling rate is so sufficiently small that for all practical purposes, weak friction does not have any impact on deviations from the thermal equilibrium population inside the well. This can be readily understood if we note that the golden-rule calculation for the activation rate to the first few excited energy levels is proportional to the dissipation strength, $\hat{\gamma}(\mu)$, whereas the time scale for decay is set by the inverse of the low temperature tunneling rate, Γ . Using as a guide the undamped, zero-temperature rate in equation 24 (which always exponentially overestimates the zero-temperature dissipative decay rate in that equation), we can expect that deviations from equation 24 occur possibly only for exponentially small friction values; that is, for

$$\hat{\gamma}(\mu)/\omega_0 \leq \Gamma(\hat{\gamma} = 0)/\omega_0 \\ = [216 E_b/(\hbar\omega_0\pi)]^{1/2} \exp\{-[36E_b/(5\hbar\omega_b)]\} \leq 10^{-6}, \quad T < T_o. \quad (33)$$

For such exponentially small friction, the tunneling rate, Γ , and the activation rate into an excited state start to compete with each other; that is, the decay rate then no longer possesses a well-defined meaning. In conclusion, unless one starts out with an externally imposed initial preparation far from thermal equilibrium, the low temperature tunneling rate in equation 24 is valid for the whole damping regime.

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^bIt can be shown that these do not exceed the classical, next higher-order correction in order of magnitude because they are proportional to $\gamma_0^{3/2}$.

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