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DECAY OF A METASTABLE STATE: A VARIATIONAL APPROXIMATION

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We consider the decay of a metastable state, coupled to a thermal reservoir, by quantum tunnelling. We calculate the leading exponential term in the W.K.B. expansion of the decay rate through a variational approximation. The approach is simple, quick and versatile, when compared with the alternative method which involves the numerical solution of non-linear, non-local, integro-differential equations. We have demonstrated the versatility of the variational approach by applying it to a few types of potentials, most of which have not been previously studied. In the few cases where numerical results are available, the variational approximation gives excellent agreement. In the cases where no numerical results are available for comparison, the variational approximation reproduces trends that are either physically reasonable or that may be inferred by interpolation between exactly soluble limits.

We also address the question: What are the effects of frequency dependent friction, or a finite noise correlation time, on the quantum tunnelling rate? This question is one that has been recently broached in the discussion of experiments on highly damped r.f. SQUIDs and Josephson junctions. We find that the effect of the memory time is to reduce the lifetime of the metastable state, towards its undamped value. Again, we find that the variational approximation reproduces the exact variation of the action to a surprisingly good degree of accuracy.

1. Introduction

The decay of a metastable state of a system in intimate contact with a thermal reservoir is a ubiquitous process in physics. At sufficiently high temperatures, the decay is conventionally considered as being activated through the occurrence of spontaneous large amplitude fluctuations of the thermal reservoir[1,2]). This picture produces decay rates which are governed by an Arrhenius type law. At low temperatures, the occur-

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rence of large amplitude thermal fluctuations becomes so seldom that other processes may be of importance in the decay. One such process is the decay by quantum tunnelling, as has been considered by Langer[3]), Callan and Coleman[4]) and others[5]). Caldeira and Leggett[6] extended these theories to include the influence of the coupling to the thermal reservoir, although they still considered only the $T = 0$ limit. This was later extended to finite temperatures by Grabert, Weiss and Hänggi[7]). It has also been shown that as the temperature is raised this finite temperature theory shows a continuous transition, at T_0, between a rate governed by quantum tunnelling to one governed by thermal activation[5a,7,8,9]). That is one recovers the high temperature form of the Arrhenius law.

In this paper, we consider the decay of a metastable state due to quantum tunneling. We show how one may calculate the dominant exponential dependence of the tunneling rate, using a variational approach. In contrast to the standard methods of calculating the rate, which involves finding the solution of a non-linear, non-local integro-differential equation, the variational approach is quick and simple. What is extremely surprising is that a simple two parameter variational ansatz produces very accurate results for the decay rate[10]). We also consider the effects of a coupling to the heat bath which are not strictly ohmic but also incorporate frequency dependent effects. These types of memory friction mechanisms have recently been proposed to be of great importance to the discussion of experiments on r.f. superconducting interference devices SQUIDs and Josephson junctions. There is experimental evidence that indicates that such effects may be present[11-14]). This could have a great effect on the tunneling rate of highly damped systems. We have, therefore, applied the variational approach to such frequency dependent damped systems, in order to ascertain the effects of a characteristic memory correlation time. We find that as the correlation time increases, the tunneling rate also increases towards the value expected for the undamped system. Since this situation has not been previously investigated, it is crucial to check the accuracy of the variational approximation. We have done so by comparing the results of the variational approximation with the asymptotic long memory-time limit which can be treated analytically. To our surprise, the variational approximation reproduces this limiting behavior exceedingly well.

In section 2, we shall outline the general formalism that we utilize to describe the quantum decay process. We closely follow the formalism as applied by Feynmann and by Langer. In section 3 we present the variational approach for the calculation of the dominant exponential part of the decay rate. We illustrate the method by applying it to decay from several potentials, most of which have not been previously considered. In the one case where numerical results exist, we check the reliability of the method. In section 4, we

consider the effect of frequency dependent friction or damping with a memory kernel. We also perform analytic calculations on the asymptotic long noise correlation-time limit to enable comparison with the results fo the variational approximation.

2. General formalism

We consider a quantum particle, which is constrained to move in a one-dimensional potential. The particle is also coupled to a thermodynamic heat bath. The heat bath is described by a set of harmonic normal modes. The coordinates of the normal modes are represented by the set φ_n, $N \geqslant n \geqslant 1$. The Lagrangian of the system is written as

$$\mathscr{L} = \frac{M}{2}\,\dot{q}^2 - V(q) + \sum_{n=1}^{N}\left[\frac{m_n}{2}\,\dot{\varphi}_n^2 - \frac{m_n}{2}\,\omega_n^2\varphi_n^2\right] - \sum_{n=1}^{N}\lambda_n\varphi_n q - \sum_{n=1}^{N}\frac{1}{2m_n}\,\frac{\lambda_n^2}{\omega_n^2}\,q^2 . \tag{2.1}$$

In this, the first two terms represent the motion of the particle of mass M in a potential $V(q)$. The third and fourth term represent the harmonic normal modes of the heat bath. The next term is a bilinear term which couples the particle to a heat bath. The last term is introduced in order that $V(q)$ coincides with the effective potential experienced by the particle.

We shall consider the decay of the particle from a metastable minimum of $V(q)$. For low temperatures, $T < T_0$, the decay rate is given by the expression[2,7,15])

$$\Gamma = \frac{2}{\hbar}\,\mathrm{Im}\,F\,, \tag{2.2}$$

in which F is given by the path integral

$$\mathrm{e}^{(-F/k_\mathrm{B}T)} = \int \mathrm{D}q(\tau)\exp\left[-\frac{S[q(\tau)]}{\hbar}\right], \tag{2.3}$$

which is to be evaluated over all closed paths that start in the metastable potential well. Furthermore, in (2.3) the closed paths must be periodic in τ, with period $\hbar/(k_\mathrm{B}T)$. The effective action in eq. (2.3) $S[q(\tau)]$ is given by[2,7,8,9])

$$S[q(\tau)] = \int_{-\hbar/2k_B T}^{\hbar/2k_B T} d\tau \left[\frac{M}{2} \dot{q}^2(\tau) + V(q) \right] + \frac{1}{2} \int_{-\hbar/2k_B T}^{\hbar/2k_B T} \int_{-\infty}^{\infty} d\tau' \, K(\tau - \tau')[q(\tau) - q(\tau')]^2 . \tag{2.4}$$

This effective action was obtained by integrating over the normal modes of the heat bath. The Lagrangian has been further simplified by analytically continuing to imaginary times, and periodically continuing the paths. The last term in (2.4) is non-local in time and represents the dynamics of the coupling to the heat bath. All the properties of the coupling between the particle and the heat bath are contained in[6])

$$K(\tau) = \int_0^{\infty} \frac{d\omega}{2\pi} J(\omega) \exp(-\omega|\tau|) , \tag{2.5}$$

where the spectral density $J(\omega)$ is given in terms of the microscopic parameters as

$$J(\omega) = \frac{\pi}{2} \sum_{n=1}^{N} \frac{\lambda_n^2}{m_n \omega_n} \delta(\omega - \omega_n) .$$

For the path integral in eq. (2.3) we use the method developed by Langer[3]) and extended by Callan and Coleman[4]). The method relies on the semiclassical approximation, where $\hbar$ is assumed to be the smallest scale. The path integral is dominated by the trajectories for which the action $S[q(\tau)]$ is stationary. These extremal trajectories are given by the solutions of

$$\frac{\delta S[q]}{\delta q} = 0 , \tag{2.6}$$

which can be re-expressed as the Euler–Lagrange equation

$$0 = -M\ddot{q}(\tau) + \frac{dV}{dq}(q(\tau)) + 2 \int_{-\infty}^{\infty} d\tau' \, K(\tau - \tau')(q(\tau) - q(\tau')) . \tag{2.7}$$

The extremal trajectories $q(\tau)$ are found by solving eq. (2.7). In the semiclassical limit, one only needs to consider the effects of paths in the immediate vicinity of the extremal trajectories.

An arbitrary periodic path $q(\tau)$ is expanded about an extremal trajectory

$\tilde{q}(\tau)$, in terms of a complete set of orthonormal functions $q_n(\tau)$,

$$q(\tau) = \tilde{q}(\tau) + \sum_n C_n q_n(\tau) \,. \tag{2.8}$$

The set of functions $\{q_n(\tau)\}$ are chosen such that the second variational derivative of the action is diagonal, to second order in the coefficients, C_n. This corresponds to requiring that $\{q_n\}$ satisfies the Hermitian eigenvalue equation

$$\left.\frac{\delta^2 S}{\delta q^2}\right|_{q=\tilde{q}} \cdot q_n = \Lambda_n q_n \,, \tag{2.9}$$

together with periodic boundary conditions

$$q_n\left(\frac{\hbar}{2k_B T}\right) = q_n\left(-\frac{\hbar}{2k_B T}\right) .$$

In the usual, semi-classical approximation only the terms in the action which are quadratic in the C_n are retained.

$$S[q(\tau)] = S[\tilde{q}(\tau)] + \sum_n \frac{\Lambda_n}{2} C_n^2 + \cdots . \tag{2.10}$$

The contributions of the small fluctuations about the extremal trajectories can be represented by integrations over the coefficients C_n. The neighborhood of each extremal trajectory contributes a term

$$\exp\left[-\frac{S[\tilde{q}(\tau)]}{\hbar}\right]\prod_n \int \frac{\mathrm{d}C_n}{(2\pi\hbar)^{1/2}} \exp\left[-\frac{\Lambda_n C_n^2}{2\hbar}\right]$$

$$= \exp\left[-\frac{S[\tilde{q}(\tau)]}{\hbar}\right]\prod_n (\Lambda_n)^{-1/2} \tag{2.11}$$

to the path integral (2.3).

For a potential with a metastable state, the Euler–Lagrange equation (2.7) has at least two trivial solutions, $q(\tau) = \text{const}$. One trivial solution corresponds to the trajectory which remains at the local metastable minimum. The other trivial solution corresponds to the trajectory which remains at the maximum of the potential barrier.

The Euler–Lagrange equation has a non-trivial solution, the so called bounce trajectory $q_B(\tau)$. This trajectory comprises a periodic path which makes an excursion from the metastable well to points on the opposite side of the potential barrier and subsequently returns to the metastable well.

The time translational invariance of the system implies that not only $q_B(\tau)$ is

an extremum of the action, but so is $q_B(\tau + \tau_0)$. Therefore, the fluctuations about the bounce trajectory must contain $\partial q_B/\partial\tau$ as a solution, with zero eigenvalue. This Goldstone-like mode restores the time translational invariance. Since the bounce trajectory is also time reversal invariant, we immediately find that $\partial q_B/\partial\tau$ contains an odd number of nodes. As has been pointed out, this implies that there exists an odd number of negative eigenvalues. Thus, the bounce will contribute an imaginary part to the path integral. On exponentiating the resulting series, one finds, with the aid of (2.2), that γ is of the form

$$\Gamma = A \exp[(S[0] - S[q_B(\tau)])/\hbar] , \tag{2.12}$$

where the prefactor A is expressed in terms of the modulus of a ratio of determinants. One crucial conclusion of this discussion is that the bounce action $S[q_B(\tau)]$ is a saddlepoint in function space, in that there exists an odd number of functions that represent directions along which the action decreases. The action increases for small excursions along the other, infinite set of directions $q_n(\tau)$. We shall make use of this property in the variational method. Another conclusion concerns the prefactor of the rate.

The prefactor A is obtained only after the series for the action, (2.10), has been terminated by neglecting terms of higher order than C_n^2. This corresponds to neglecting terms of the action of higher order than $\hbar$. This truncation of the series is only justified if it is rapidly convergent. Under such circumstances, the rate is dominated by the exponential term. Therefore, we shall calculate the rate in the form

$$\ln \Gamma = -(S_B - S_0)/\hbar , \tag{2.13}$$

where S_B is the action calculated for the bounce trajectory and S_0 is the trivial trajectory corresponding to the minimum of the metastable potential.

Only in a few special cases, it has been possible to find exact analytic solutions for $q_B(\tau)$, and to find the action[9,16]). Likewise, numerical solutions[17,18]) have only been obtained in the case of a cubic potential and ohmic dissipation

$$J(\omega) = M\eta\omega . \tag{2.14}$$

Therefore, in the next section, we shall present a method which enables the approximate calculation of S_B for many different types of potentials and dissipative mechanisms. The method is expected to be useful since it is both extremely simple, and gives surprisingly accurate results.

3. The variational approximation

In this section we shall describe the variational approximation and apply it to the problem of decay from a metastable potential, in the presence of ohmic dissipation. We shall consider potentials $V(q)$ of the form

$$V(q) = \frac{M\omega_0^2}{2} q^2\left(1 - \left(\frac{q}{\Delta q}\right)^n\right), \tag{3.1}$$

in which n is an odd integer. In this section, we shall restrict our attention to the case of ohmic dissipation (eq. (2.14)). The accuracy of our approximation will be assessed by comparison with numerical results, which only exist for the cubic potential, where $n = 1$. We compare our results both with the $T = 0$ values of Chang and Chakravarty[17]) as well as the finite temperature values computed by Grabert, Olschowski and Weiss[18]).

The action, evaluated along the bounce trajectory, is a saddle-point in the space defined by the set C_n. We propose to evaluate this saddle-point action, approximately, by a direct variational method.

We shall introduce a family of trial trajectories, which hopefully are close to the exact solution. The trial trajectories only depends on a small set of parameters $\{\alpha_i\}$. The values of the parameters are chosen such that the corresponding action is extremalized, and is also a saddle-point. The resulting action is our variational approximation to S_B. Thus, we merely have restricted the variational principle for S_B onto a subset of the full functional space. As the family of trial functions is appropriately enlarged, one would expect that the variational approximation should approach S_B more closely.

Caldeira and Leggett have introduced a second functional[6]), defined for a specific class of bounce trajectories and potentials in order to show that the bounce action is a monotonically increasing function of the strength of the dissipation. We prove this directly in appendix A. The second functional defined by Caldeira and Leggett, produces an upper bound to the bounce action. When the family of trial functions that we consider lies within the class considered by Caldeira and Leggett, our variational approximation to the bounce action coincides with the value of their second functional and provides an upper bound to the bounce action.

We shall introduce the family of trial trajectories

$$q(\tau) = \frac{a}{1 - b\cos(2\pi k_B T\tau/\hbar)}, \tag{3.2}$$

which depends on the two parameters a and b. These trajectories start at the point $q = a/(1 + b)$ inside the metastable well, and at $\tau = 0$ reach the point

$q = a/(1-b)$ outside the potential barrier and then subsequently return to the starting point. The choice of the finite temperature variational ansatz (3.2) is motivated by the following considerations:

i) $q(\tau)$ has period $\hbar/k_B T$;

ii) $q(\tau)$ reduces to the exact extremal trajectory for temperatures in the vicinity of the cross-over to thermal activation, $T \lesssim T_0$;

iii) $q(\tau)$ reduces to the asymptotically exact bounce trajectory in the limit $\alpha = (\eta/2\omega_0) \to \infty$, for the cubic potential.

We then evaluate the action along the trial trajectory (3.2). We find that the action is given by the expression

$$\frac{S_n(a,b)}{M\omega_0(\Delta q)^2} = \frac{\hbar\omega_0}{2k_B T}\left[y^2\left(\frac{2\pi k_B T}{\hbar\omega_0}\right)^2 \frac{x}{2}(x^2-1) + \left(\frac{2\pi k_B T}{\hbar\omega_0}\right)\alpha y^2(x^2-1) + y^2 x - y^{n+2}P_{n+1}(x)\right], \tag{3.3}$$

where $y = a/\Delta q\sqrt{1-b^2}$, $x = 1/\sqrt{1-b^2}$ and the $P_n(x)$ are Legendre polynomials. The first term in the square brackets represents the kinetic energy, the third and forth terms represent the non-linear potential, while the second term represents the effect of the dissipation: $\alpha = \eta/(2\omega_0)$.

The extremal conditions can be rewritten as $\partial S/\partial x = \partial S/\partial y = 0$. These have two solutions, one is the trivial solution $y = 0$ which corresponds to the trajectory remaining at the metastable minimum, and the other solution can be written as

$$y^n = \frac{1}{n+2}\frac{1}{P_{n+1}(x)} \times \left\{2\alpha\left(\frac{2\pi k_B T}{\hbar\omega_0}\right)(x^2-1) + \left(\frac{2\pi k_B T}{\hbar\omega_0}\right)^2 x(x^2-1) + 2x\right\}, \tag{3.4}$$

where x is given by the root of the equation

$$\frac{1}{n+2}\frac{\mathrm{d}}{\mathrm{d}x}\ln P_{n+1}(x)\left[2\alpha\left(\frac{2\pi k_B T}{\hbar\omega_0}\right)(x^2-1) + \left(\frac{2\pi k_B T}{\hbar\omega_0}\right)^2 x(x^2-1) + 2x\right] = \left[\left(\frac{2\pi k_B T}{\hbar\omega_0}\right)^2 \frac{1}{2}(3x^2-1) + 2\alpha\left(\frac{2\pi k_B T}{\hbar\omega_0}\right)x + 1\right]. \tag{3.5}$$

This is equivalent to an algebraic equation of order $n+3$.

For the cubic potential this results in a quartic equation, at finite tempera-

tures. For $T = 0$, as we shall see later, everything simplifies and the corresponding equation is a quadratic equation.

Eq. (3.5) can be shown to possess a root for $1 \leqslant x \leqslant \infty$ in the temperature range $0 \leqslant T \leqslant T_0$, where

$$T_0 = \frac{\hbar \omega_0}{2\pi k_B} \{\sqrt{\alpha^2 + n} - \alpha\} . \tag{3.6}$$

That is, one finds a variational approximation for the action for all temperatures in the region where quantum tunnelling is the dominant decay mechanism.

At the temperature $T = T_0$, where the cross-over between thermal activation and quantum tunnelling occurs, we find that $x = 1$, and

$$y^n = \frac{2}{n+2} . \tag{3.7}$$

The trial trajectory becomes exact, and remains at the top of the potential barrier. The action is then given by $\hbar V_{max}/k_B T$ where V_{max} is the height of the potential barrier, which is given by

$$V_{max} = \frac{M\omega_0^2}{2} (\Delta q)^2 \frac{n}{n+2} \left[\frac{2}{n+2}\right]^{2/n} . \tag{3.8}$$

Thus the action matches smoothly onto the Arrhenius factor[7]), and is in agreement with the exact results of Grabert and Weiss[8]).

At arbitrary temperatures, the polynomial equation (3.5) is solved numerically. The results of this finite temperature variational approximation can be compared with the numerical values calculated by Grabert, Olschowski and Weiss for the cubic potential ($n = 1$) [18]). These are shown in table I. The action is expressed in units of $M\omega_0 \Delta q^2$. The results are tabulated for various values of α and temperature ratio's T/T_0.

The agreement between the variational results and the numerical values is exceptionally good for large and intermediate values of the damping strength α. The largest discrepancy occurs for the undamped case ($\alpha = 0$) at $T/T_0 = 0.4$.

We note that our approximate values of the action are greater than the numerical values. Since our variational ansatz (3.2) is of the class considered by Caldeira and Leggett, our results are in agreement with the minimum principle that they proposed.

In the $T = 0$ limit, one must handle the limiting procedure with care, since both $b \to 1$ and $a \to 0$. It is convenient to introduce the parameterization

Table I
The dimensionless action $S/(M\omega_0 \Delta q^2)$ for the potential $n = 1$. The action is given for various values of the dimensionless damping strengths α and reduced temperatures T/T_0. The results of the variational approximation (V.A.) are presented alongside the numerical results obtained by Grabert, Olschowski and Weiss (Ref. 18).

T/T_0	0.1		0.4		0.6		0.8	
α	V.A.	Ref. 18	V.A.	Ref. 18	V.A.	Ref. 18	V.A.	Ref. 18
0.00	0.567	0.533	0.583	0.533	0.577	0.533	0.540	0.521
0.05	0.612	0.580	0.623	0.577	0.611	0.570	0.568	0.551
0.10	0.659	0.629	0.664	0.621	0.647	0.610	0.599	0.583
0.50	1.070	1.052	1.036	1.015	0.978	0.963	0.885	0.874
1.00	1.656	1.644	1.581	1.570	1.477	1.467	1.324	1.319
2.00	2.942	2.941	2.796	2.793	2.601	2.600	2.326	2.326
4.00	5.65	5.65	5.37	5.37	4.99	4.99	4.46	4.46
10.00	13.95	13.93	13.25	13.26	12.32	12.30	11.01	11.04

$$\tilde{b} = \frac{2\pi k_B T}{\hbar} \frac{1}{\sqrt{1 - b^2}} \tag{3.9a}$$

and

$$\tilde{a} = \frac{a}{1 - b} . \tag{3.9b}$$

The variational ansatz can be seen to reduce to the Lorentzian

$$q(\tau) = \frac{\tilde{a}}{1 + \tilde{b}^2 \tau^2} \tag{3.10}$$

at $T = 0$. We find that

$$\tilde{a} = \frac{4}{3} \Delta q \left(1 - \frac{\tilde{b}^2}{2\omega_0^2}\right), \tag{3.11a}$$

$$\tilde{b} = \frac{\eta}{5} \left\{ \sqrt{1 + 10 \frac{\omega_0^2}{\eta^2}} - 1 \right\}, \tag{3.11b}$$

for the case $n = 1$.

The corresponding approximate action is given by

$$S(\tilde{a}, \tilde{b}) = \frac{\pi M \tilde{a}^2}{8} \left[\tilde{b} + \frac{2\omega_0^2}{\tilde{b}} \left(1 - \frac{3\tilde{a}}{4\Delta q}\right) + \eta \right], \quad T = 0 . \tag{3.12}$$

The results are shown in table II. They can be directly compared with the numerical results of Chang and Chakravarty[17]). We see that the worst discrepancy occurs for $\alpha = 0$. This case is exactly soluble, and we find that our approximation gives a value which is 5.9% larger than the exact analytic value. The error decreases as α increases. For $\alpha = 1.1746$ our approximation gives a result 0.95% above the exact analytical result of Riseborough, Hänggi and Freidkin[16]). By contrast, the value obtained by interpolating between the numbers given by Chang and Chakravarty differs by 0.67% from the exact value. For even larger values of α, the discrepancies are negligible.

There have been no numerical studies of potentials other than $n = 1$. Therefore, we are unable to extensively assess the accuracy of our approximation. The results for the action are tabulated in table III for the $n = 3$ case and in table IV for the $n = 5$ case. The action is given in units of $M\omega_0 \Delta q^2$.

In order to compare our results with exact values, we have found the $\alpha = 0$ and $T = 0$ bounce trajectory

$$q(\tau) = \Delta q \operatorname{sech}^{2/n}\left(\frac{n\omega_0 \tau}{2}\right), \tag{3.13}$$

and its corresponding action

Table II
The dimensionless action $S/(M\omega_0 \Delta q^2)$ for the potential $n = 1$ at zero temperature for various damping strengths α. The results of the variational approximation (see 3.12) are given in the column denoted by V.A., alongside the numerical results by Chang and Chakravarty (Ref. 17).

α	V.A.	Ref. 17
0.00	0.565	0.533
0.01	0.574	0.543
0.05	0.611	0.581
0.10	0.657	0.629
0.50	1.072	1.055
1.00	1.661	1.651
1.50	2.295	2.288
2.00	2.951	2.947
2.50	3.622	3.617
3.00	4.300	4.296
3.50	4.983	4.979
4.00	5.670	5.665
10	13.997	13.986

Table III
The action S_3 in units of $(M\omega_0 \Delta q^2)$ for various damping strengths α and temperatures T/T_0. The action is calculated variationally with the potential (3.1) with $n = 3$.

α \ T/T_0	0.1	0.4	0.6	0.8
0.00	0.750	0.758	0.739	0.686
0.05	0.791	0.791	0.766	0.708
0.10	0.831	0.825	0.794	0.730
0.50	1.177	1.118	1.038	0.927
1.00	1.648	1.532	1.392	1.219
2.00	2.673	2.466	2.206	1.901
4.00	4.876	4.509	4.015	3.433
10.00	11.779	10.926	9.718	8.286

Table IV
The variational approximation for the effective action S_5 for the potential in (3.1) where $n = 5$. The action is given in units of $(M\omega_0 \Delta q^2)$ for a set of dimensionless damping strengths α and reduced temperatures T/T_0.

α \ T/T_0	0.1	0.4	0.6	0.8
0.00	0.824	0.823	0.788	0.715
0.05	0.863	0.853	0.811	0.732
0.10	0.902	0.883	0.834	0.750
0.50	1.226	1.143	1.038	0.906
1.00	1.659	1.503	1.324	1.129
2.00	2.588	2.310	1.978	1.650
4.00	4.580	4.102	3.546	2.845
10.00	10.876	9.811	8.211	6.725

$$S_n = M\omega_0(\Delta q)^2 \frac{2^{4/n}}{n+4} \frac{\Gamma^2(2/n)}{\Gamma(4/n)}, \tag{3.14}$$

where $\Gamma(z)$ is the gamma function.

On comparing our approximate results with the exact $\alpha = 0$ and $T = 0$ values, we find that for $n = 3$ the variational approximation yields a value which is 1.3% too large. This discrepancy is decreased for $n = 5$, where we find that our value is only 0.6% too large.

The trends exhibited in tables III and IV can be summarized as follows: The effect of increasing n is to increase the undamped value of the action. This is

easily understood since increasing n merely corresponds to increasing the height of the potential barrier. On the other hand, increasing n does result in a decrease of the action calculated with large α-values. This decrease may also be inferred from comparison of the exact solution for large α with $n = 1$, and the $n \to \infty$ limit. For $n \to \infty$, one finds

$$\lim_{n\to\infty} \frac{S_n}{M\omega_0(\Delta q)^2} = \frac{\pi}{2}\,\frac{\alpha}{\ln \alpha}\,, \qquad T = 0\,, \quad \alpha \gg 1\,, \tag{3.15}$$

while for $n = 1$,

$$\lim_{\alpha\to\infty} \frac{S_1}{M\omega_0(\Delta q)^2} = \pi\,\frac{4}{9}\,\alpha\,, \qquad T = 0\,, \quad \alpha \gg 1\,. \tag{3.16}$$

Thus one is led to expect that S_n should decrease, for large α, as one increases n. Therefore, the variational approximation does lead to reasonable results.

In the next section, we shall consider couplings to the heat bath which do not give rise to strictly ohmic dissipation described by (2.14). In particular, we shall assess the effect of introducing a characteristic relaxation time into the heat bath spectral density.

4. Frequency dependent friction

There exists considerable experimental evidence that Josephson junctions and r.f. superconducting quantum interference devices (S.Q.U.I.D.s) cannot be completely described by the phenomenological Resistively Shunted Junction (R.S.J.) model. These experiments indicate that at sufficiently high frequencies the effective resistivity in the R.S.J. model is frequency dependent. The T^2 dependence observed in the logarithm of the tunneling rate in these systems[11,12]) is, however, characteristic of ohmic friction. Therefore, it may be reasonable to investigate models in which the spectral density $J(\omega)$ is ohmic at low frequencies and deviates from the $(M\eta\omega)$-behavior *at high frequencies*. This leads to a frequency-dependent friction or memory damping[2]). In this section, we shall apply the variational approximation to such a case. This application serves a two-fold purpose. First, it will show the types of effects that memory damping has on quantum mechanical tunneling, a subject that has not been extensively studied. Secondly, the application will display the versatility and the accuracy of the variational approximation to novel situations.

Let us consider the case of frequency dependent ohmic damping, where the spectral density $J(\omega)$ is given by

$$J(\omega) = M\eta \frac{\omega}{1 + \omega^2 \tau_0^2}, \tag{4.1}$$

in which τ_0 is a Drude cut-off. This type of damping corresponds to the damping that appears in the phenomenological classical equation

$$M\ddot{q}(\tau) + \int_0^\tau \frac{M\eta}{\tau_0} \exp\left[-\frac{(\tau - \tau')}{\tau_0}\right] \dot{q}(\tau')\, \mathrm{d}\tau' + \frac{\mathrm{d}V[q(\tau)]}{\mathrm{d}q} = 0. \tag{4.2}$$

The Drude cut-off form of ohmic damping gives rise to a dissipative term in the action as in eq. (2.4), but where

$$K(\tau) = \frac{M\eta}{2\pi\tau_0^2} g\left(\frac{\tau}{\tau_0}\right), \tag{4.3}$$

in which $g(x)$ is the auxiliary exponential integral function[19]). As τ_0 tends to zero, this form of $K(\tau)$ reduces to the $1/\tau^2$ dependence found with purely ohmic damping. We note that increasing τ_0, monotonically decreases the magnitude of $K(\tau)$.

We evaluate the action with the variational ansatz (3.2). The kinetic and potential parts of the action are of the same form as previously evaluated in eq. (3.3). Only the form of the dissipative part, proportional to α, will be changed. This latter term is replaced by

$$M\omega_0(\Delta q)^2 4\pi\alpha y^2 \sum_{m=1}^{\infty} \left[\frac{m}{1 + m(2\pi k_B T\tau_0/\hbar)} \left\{\frac{x-1}{x+1}\right\}^m\right], \tag{4.4}$$

which can be written as a hypergeometric function.

The total action is extremalized by

$$\frac{\partial S}{\partial x} = 0, \quad \frac{\partial S}{\partial y} = 0. \tag{4.5}$$

These equations can, as before, be reduced to one equation. The resulting equation is solved numerically.

The cross-over temperature T_0, below which the decay is dominated by quantum tunneling, is given by the root of the cubic equation

$$\left(\frac{2\pi k_B T_0}{\hbar\omega_0}\right)^3 + \left(\frac{2\pi k_B T_0}{\hbar\omega_0}\right)^2 \frac{1}{\omega_0\tau_0} + \left(\frac{2\pi k_B T_0}{\hbar\omega_0}\right)\left(\frac{2\alpha}{\omega_0\tau_0} - n\right) - \frac{n}{\omega_0\tau_0} = 0, \tag{4.6}$$

which has just one positive root.

At the cross-over temperature, one recovers the exact bounce trajectory. The resulting action gives rise to the expected exponential Arrhenius form of the decay rate.

In fig. 1, we plot the action for the cubic potential as a function of $\omega_0\tau$. The three curves represent the three α values of 10, 4 and 1. The temperature ratio T/T_0 is fixed at 0.1. We see that as $\omega_0\tau_0$ is increased, the action is reduced towards its undamped value. We shall examine this approach to the undamped case in greater detail, since it provides a further quantitative test of the variational approximation.

Using the variational approximation we find that the quantity

$$\frac{\omega_0\tau_0}{\alpha}\,[S(\alpha, T) - S(0, T)]$$

is a function of temperature alone, for large $\omega_0\tau_0$. The value of this function at $T = 0$ is found to be 2.71 ± 0.06, while direct analytical calculation yields this constant as 2.67. These calculations are presented in appendix B. Thus we see, the variational approximation not only reproduces the correct variation of the action with $\omega_0\tau_0$, for large $\omega_0\tau_0$, but also does very well in the determination of the constant of proportionality.

In figs. 2 and 3 we plot the action as a function of $\omega_0\tau_0$ for the potentials with

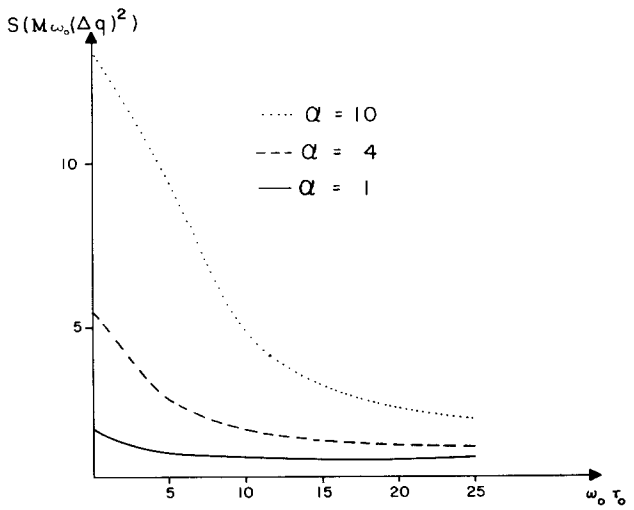

Fig. 1. The effective action S, for the non-ohmic dissipation (4.1) in units of $(M\omega_0\,\Delta q^2)$, is depicted for the cubic potential ($n = 1$), versus the dimensionless correlation time $\omega_0\tau_0$ of the memory-damping, at fixed reduced temperature $T/T_0 = 0.1$. The different curves correspond to different values of the dimensionless zero-frequency damping $\alpha = \eta/2\omega_0$ shown in the figure.

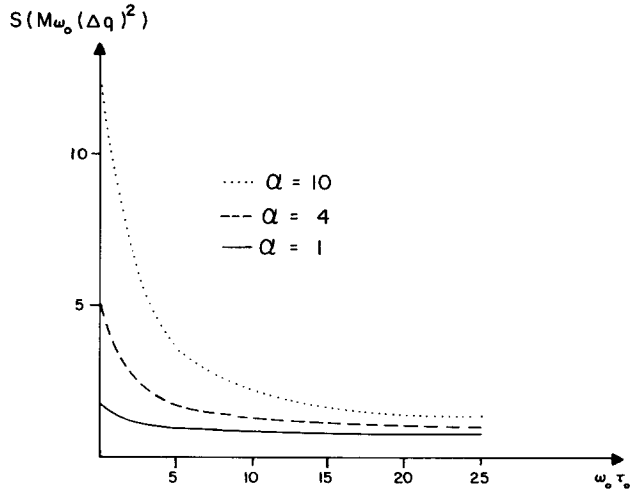

Fig. 2. Non-ohmic effective action S versus dimensionless memory-correlation time $\omega_0\tau$ for the potential in (3.1) with $n = 3$. The reduced temperature is kept fixed at $T/T_0 = 0.1$. The three curves correspond to different zero-frequency damping strengths α shown in the figure.

$n = 2$ and 5, respectively. The curves represent three values of $\alpha = 10$, 4 and 1; the reduced temperature $T/T_0 = 0.1$ is maintained constant. Again we note that as $\omega_0\tau_0$ is increased, the action reduces towards the undamped value. The approach to this value is again dominated by the variation

$$S_n(\alpha, T) - S_n(\alpha, 0) \simeq \frac{\alpha}{\omega_0\tau_0} f\left(\frac{T}{T_0}\right)$$

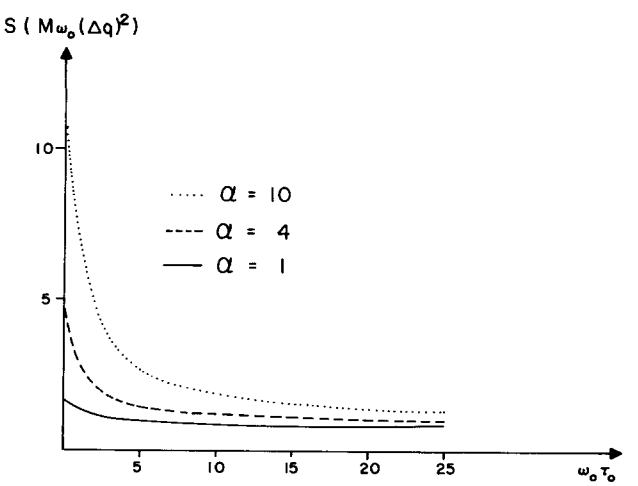

Fig. 3. The same as in fig. 2 for the potential (3.1) with $n = 5$.

for large $\omega_0\tau_0$. In this expression, f is a universal function of T/T_0. This is in agreement with the variation derived in appendix B.

To summarise, we see that the effect of introducing a characteristic time scale into the spectral density of the thermal reservoir has the effect of reducing the action, and therefore increasing the decay rate. We see that the variational approximation reproduces the exact asymptotic large $(\omega_0\tau_0)$-variation of the action to a surprisingly high degree of accuracy.

5. Conclusions

We have utilized a variational approach to calculate the rate of decay from a metastable state, due to quantum tunnelling. The variational approach calculates the leading term in the W.K.B. expansion of the tunnelling rate.

The main advantage of the variational approach is that for systems which are coupled to a heat bath: The standard path integral (W.K.B.) approach would require one to solve a non-linear, non-local in time, integro-differential equation. This can only be performed numerically, in all but a few special cases. The resulting numerical data has then to be integrated to produce the leading dependence of the decay rate. The variational approach is particularly simple and quick. This is best illustrated by comparing the numerical procedure used by Chang and Chakravarty to be $T = 0$, $n = 1$ decay problem with the variational results contained in eqs. (3.11) and (3.12), obtained by solving a quadratic equation. What is most surprising is the accuracy of the results obtained by the variational method. For values of $\alpha > 1$, we see that the accuracy we obtain is comparable to those obtained numerically by Chang and Chakravarty[17]). At finite temperatures, the variational approach also closely follows the numerical results for the $n = 1$ case obtained by Grabert, Olschowski and Weiss[18]).

The variational method may be extremely useful in providing quick and simple calculations of the decay rate for novel physical situations. To demonstrate this we have addressed potentials, $n = 3$ and $n = 5$, for which numerical results are not available. The variational approximation has closely reproduced the known exactly soluble limits, again with surprisingly good accuracy. It has also been able to give the trends which can be inferred from physical considerations.

Finally, we have also addressed a question of some physical importance. Namely, what effect does a frequency dependent friction have on the rate of decay by quantum tunnelling? This question has been raised since the experimental measurements on r.f. SQUIDs and Josephson junctions seem to

indicate that the effective resistivity in the R.S.J. model should be frequency dependent. Furthermore, this frequency dependence has been invoked to provide a mechanism which might explain a possible discrepancy between theory and experiment on highly damped SQUIDs [12]). The variational method has shown that the influence of a characteristic time in the friction can produce a significant increase in the tunnelling rate. The tunnelling rate approaches the undamped tunnelling rate, as the characteristic memory correlation-time increases. This asymptotic approach to the undamped tunnelling rate is accurately reproduced by the variational approximation. Furthermore, as the temperature approaches the cross-over between quantum tunnelling and thermal activation, the variational approach becomes exact. At the cross-over temperature one recovers the results obtained by Hänggi et al.[20]) on the effect of the characteristic time-scale on the cross-over temperature.

In summary, the variational approach is simple, varsatile and produces surprisingly good results for the leading dependence of the decay rate.

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Appendix A

The bounce action is a monotonically increasing function of the dissipation strength α. This may be proved quite simply and directly. First, we shall consider the change in the bounce action, if α is changed to $\alpha + \mathrm{d}\alpha$. Under such a change the *bounce* trajectory will alter by an amount δq. To lowest order in $\delta\alpha$, we find that

$$S(q + \delta q, \alpha + \mathrm{d}\alpha) - S(q, \alpha) = \int \left(\frac{\delta S}{\delta q}\right) \delta q(\tau)\, \mathrm{d}\tau + \left(\frac{\partial S}{\partial \alpha}\right) \mathrm{d}\alpha \,.$$

Since $(\delta S/\delta q) = 0$, this is equal to $(\partial S/\partial \alpha)\, \mathrm{d}\alpha$. The only explicit α-dependence occurs through the dissipation term, which for ohmic dissipation is positive definite. Therefore, we find

$$\left(\frac{\partial S}{\partial \alpha}\right) > 0 \,,$$

which holds for any value of α. Thus the bounce action is a monotonically increasing function of α.

Appendix B

The asymptotic long memory time limit $\omega_0\tau_0 \gg 1$

We shall consider the Euler–Lagrange equation with memory damping,

$$\ddot{q}(\tau) - \omega_0^2 q(\tau)\left[1 - \frac{n+2}{2}\left(\frac{q}{\Delta q}\right)^n\right] = 2\int_{-\infty}^{\infty} d\tau'\, K(\tau-\tau')[q(\tau) - q(\tau')]\,, \tag{B.1}$$

where the damping kernel is

$$K(\tau) = \frac{\eta}{2\pi\tau_0^2}\, g\left(\frac{\tau}{\tau_0}\right),$$

as defined in eq. (4.3).

For large $\omega_0\tau_0$ and $\alpha/\omega_0\tau_0 \ll 1$, we may linearize the solution

$$q(\tau) = q_0(\tau) + \varphi(\tau)\,, \tag{B.2}$$

in which $q_0(\tau)$ is the undamped bounce trajectory. The $T = 0$ form of $q_0(\tau)$ is given in eq. (3.13).

The function $\varphi(\tau)$ is assumed to be small compared with $q_0(\tau)$. In the linear approximation, $\varphi(\tau)$ is found from the equation

$$\frac{d^2\varphi}{dy^2} - \varphi + \frac{(n+1)(n+2)}{2}\operatorname{sech}^2\left(\frac{ny}{2}\right)\varphi$$

$$= \frac{2}{\pi}\,\frac{\alpha}{(\omega_0\tau_0)^2}\int_{-\infty}^{\infty} dy'\, g\left(\frac{y-y'}{\omega_0\tau_0}\right)\left[q_0\left(\frac{y}{\omega_0}\right) - q_0\left(\frac{y'}{\omega_0}\right)\right], \tag{B.3}$$

where $y = \omega_0\tau$. The function $\varphi(\tau)$ must be an even-function of τ, and satisfy the boundary conditions

$$\lim_{|\tau|\to\infty} \varphi(\tau) = 0\,. \tag{B.4}$$

The inhomogeneous term in eq. (3) can be rewritten as

$$\frac{2\alpha}{\omega_0\tau_0}\, q_0\left(\frac{y}{\omega_0}\right) - \frac{2\alpha}{(\omega_0\tau_0)^2}\int_0^\infty \mathrm{d}p\, \frac{C\left(\frac{p}{\omega_0\tau_0}\right)\cdot 2\cos\frac{py}{\omega_0\tau_0}}{1+p}\,, \tag{B.5}$$

where

$$C(p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-ipy}\, q_0\left(\frac{y}{\omega_0}\right)\mathrm{d}y$$

is that Fourier transform of the bounce. In the limit $\omega_0\tau_0 \gg 1$, the second term can be shown to be negligible in comparison to the first term. On using the general method for solving linear inhomogeneous differential equations one can find $\varphi(\tau)$. The function $\varphi(\tau)$ is then proportional to $\alpha/\omega_0\tau_0$ for large $\omega_0\tau_0$.

The action for the $T = 0$ bounce is given by

$$S_n(\alpha, 0) = \frac{nM\omega_0^2}{4}(\Delta q)^2 \int_{-\infty}^{\infty} \mathrm{d}\tau \left(\frac{q(\tau)}{\Delta q}\right)^{n+2}. \tag{B.6}$$

On substitution of the form of $q(\tau)$ given by (B.2) we find that the leading correction to the undamped action is given by

$$S_n(\alpha, 0) - S_n(0, 0) = M\omega_0^2(\Delta q)^2\, \frac{n(n+2)}{4} \times \int_{-\infty}^{\infty} \mathrm{d}\tau \left[\operatorname{sech}\frac{n\omega_0\tau}{2}\right]^{2(n+1)/n} \frac{\varphi(\tau)}{\Delta q}\,. \tag{B.7}$$

Thus, we find that

$$\frac{S_n(\alpha, 0) - S_n(0, 0)}{M\omega_0(\Delta q)^2} \sim \frac{\alpha}{\omega_0\tau_0} \ll 1\,, \tag{B.8}$$

since $\varphi(\tau)/\Delta q \sim \alpha/\omega_0\tau_0$.

The constant of proportionality is found by direct calculation.

For example, with $n = 1$, we find that

$$\frac{\varphi(\tau)}{\Delta q} = \frac{\alpha}{\omega_0\tau_0}\left(1 - \frac{\omega_0\tau}{2}\tanh\frac{\omega_0\tau}{2}\right)\operatorname{sech}^2\frac{\omega_0\tau}{2}\,, \tag{B.9}$$

which results in the expression

$$S(\alpha,0)-S(0,0)=\frac{3}{4}M\omega_0^2(\Delta q)^2\left(\frac{\alpha}{\omega_0\tau_0}\right)$$
$$\times\int_{-\infty}^{\infty}\mathrm{d}\tau\,\mathrm{sech}^6\frac{\omega_0\tau}{2}\left(1-\frac{\omega_0\tau}{2}\tanh\frac{\omega_0\tau}{2}\right), \tag{B.10}$$

which is evaluated as

$$\frac{S(\alpha,0)-S(0,0)}{M\omega_0(\Delta q)^2}=\frac{8}{3}\frac{\alpha}{\omega_0\tau_0}. \tag{B.11}$$

This is to be compared with the variation of

$$(2.71\pm0.06)\frac{\alpha}{\omega_0\tau_0}$$

obtained by the variational approximation, as described in the text.

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