Decay of a metastable state: A variational approach

E. Freidkin, Peter Riseborough, and Peter Hanggi
Department of Physics, Polytechnic Institute of New York, 333 Jay Street, Brooklyn, New York 11201
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We evaluate the exponential suppression of the quantum tunneling rate due to the coupling with a thermal reservoir. The exponential dependence is calculated by a variational method, in which an approximate saddle point of the effective action is found. The effect of finite temperatures is accounted for. We calculate the exponential part of the rate for several potentials, some of which have not been considered previously. The method gives excellent agreement with numerically calculated values, where they exist. We also consider the effect of Ohmic damping mechanisms of Drude form (memory damping). This latter case may be of importance for experiments on rf superconducting quantum interference devices and Josephson junctions where frequency-dependent damping mechanisms have been observed. The trends exhibited by the variational approximation can be understood qualitatively on the basis of physical arguments.

The decay of a metastable state by quantum tunneling is strongly affected by the coupling to a heat bath[1] and by temperature.[2-4] The decay rate has been shown to be of the form[1-8]

$$\Gamma = A\exp[-S/\hbar]\ ,$$

where S is the effective action

$$S=\int_{-1/2T}^{1/2T} d\tau\left[\frac{M}{2}\left(\frac{dq}{d\tau}\right)^2+V(q)\right] +\tfrac{1}{2}\int_{-1/2T}^{1/2T} d\tau P\int_{-\infty}^{\infty} d\tau' k(\tau-\tau')[q(\tau)-q(\tau')]^2\ , \tag{1a}$$

evaluated along the extremal trajectory (P denotes principal value). The last term in the action represents the coupling to the heat bath.[1] The path $q(\tau)$ satisfies the boundary conditions

$$q\left(\tau+\frac{1}{2T}\right)=q\left(\tau-\frac{1}{2T}\right)\ . \tag{1b}$$

The particular choice $k(\tau)$

$$k(\tau)=\frac{M\eta}{2\pi}\left(\frac{1}{\tau^2}\right) \tag{2}$$

has been shown to correspond to Ohmic damping.[1] The usual procedure for calculating the decay rate entails the solving of the Euler-Lagrange equation for the trajectory, which is a saddle point of the action. However, in the presence of damping the Euler-Lagrange equation is not only nonlinear, but also nonlocal in time. Therefore, analytic solutions have only been found in a few special cases.[1,3,8] Numerical solutions have been found at $T=0$ by Chang and Chakravarty,[5] and at finite temperatures by Grabert, Olschowski, and Weiss[6] for the case of a cubic potential.

In this note, we shall show that the extremal action S can be found quite accurately and directly by a variational method. The saddle point of the action shall be found approximately by truncating the full space of functions onto a subset, i.e., a family of trial trajectories. The approximate action is given by the saddle-point value. We shall use the two-parameter variational ansatz

$$q(\tau)=\frac{a}{1-b\cos(2\pi T\tau)}\ . \tag{3}$$

This particular functional form is motivated by the following points: (i) $q(\tau)$ has period $1/T$. (ii) $q(\tau)$ reduces to the exact extremal trajectory in the vicinity of the temperature, at which the rate crosses over from quantum tunneling to thermal activation.[2,4,7,8] (iii) $q(\tau)$ reduces to the asymptotically exact trajectory in the overdamped limit for the cubic potential.[8] We shall consider the decay out of the $q=0$, metastable minima of the family of potentials

$$V(q)=\frac{M\omega_0^2q^2}{2}\left[1-\left(\frac{q}{\Delta q}\right)^n\right] \tag{4}$$

in which n is an odd integer. Only the case corresponding to $n=1$ has been studied previously. We evaluate the action S_n [Eq. (1)] with this form of $V(q)$ and $k(\tau)$ given by Eq. (2). On substitution of the trial trajectory [Eq. (3)], we obtain

$$\frac{S_n}{M\omega_0\Delta q^2}=\left(\frac{\omega_0}{2\pi T}\right)\left[y^2\left(\frac{2\pi T}{\omega_0}\right)^2\frac{x}{2}(x^2-1) +\alpha y^2\left(\frac{2\pi T}{\omega_0}\right)(x^2-1) +y^2x-y^{n+2}P_{n+1}(x)\right]\ , \tag{5}$$

where

$$y=\frac{a}{\Delta q}\frac{1}{\sqrt{1-b^2}},\quad x=\frac{1}{\sqrt{1-b^2}},\quad \alpha=\left(\frac{\eta}{2\omega_0}\right)$$

and the $P_m(x)$ are the Legendre polynomials.

The extremal conditions $\partial S/\partial a=0$ and $\partial S/\partial b=0$ have a nontrivial solution. These conditions can be reformulated as

$$(n+2)y^nP_{n+1}(x)=2\left[\left(\frac{2\pi T}{\omega_0}\right)^2\frac{x}{2}(x^2-1)+\alpha\left(\frac{2\pi T}{\omega_0}\right)(x^2-1)+x\right], \tag{6}$$

from which y can be obtained immediately. The remaining condition can be rewritten as

$$\frac{2}{n+2}\left(\frac{d}{dx}\ln P_{n+1}(x)\right)\left[\left(\frac{2\pi T}{\omega_0}\right)^2\frac{x}{2}(x^2-1)+\alpha\left(\frac{2\pi T}{\omega_0}\right)(x^2-1)+x\right]=\left[\left(\frac{2\pi T}{\omega_0}\right)^2(3x^2-1)/2+2\alpha\left(\frac{2\pi T}{\omega_0}\right)x+1\right]. \tag{7}$$

This is equivalent to an algebraic equation of order $n+3$. This equation always has a nontrivial solution for temperatures in the range

$$T_0 \geq T \geq 0 ,$$

where

$$T_0=\frac{\omega_0}{2\pi}(\sqrt{\alpha^2+n}-\alpha) \tag{8}$$

is the crossover temperature to thermal activation.[2-4,7,8]

For the case where $n=1$, the results of this variational procedure can be compared directly with the numerical values of Grabert, Olschowski, and Weiss.[6] The results are shown in Table I. The action is expressed in units of $M\omega_0\Delta q^2$, and the temperature in terms of T_0. It should be noted that in the original units used in Ref. 6 the values only have three significant digits. We see that for intermediate-to-large damping values (α) the variational approximation agrees excellently with the numerical values. Note that the variational approximation gives results which are equal to, or higher than the numerical values[9] (within the numerical accuracy). Furthermore, as the temperature T/T_0 approaches unity, the results become exact. The worst error occurs at low temperature for the undamped case. This limit is exactly soluble, and we find that the total error is less than 6%.

In Tables II and III we present the results for $n=3$ and $n=5$, respectively. In these cases the only results that are available for comparison are those at the crossover temperature T_0, and the value of the $\alpha=0$, $T=0$ action S_n which is calculated as

$$\frac{S_n}{M\omega_0\Delta q^2}=\frac{2^{4/n}}{n+4}\frac{\Gamma^2(2/n)}{\Gamma(4/n)} . \tag{9}$$

We see that the low-damping low-temperature limit of the variational approximation is just 1.3% above the exact result for $n=3$, and the corresponding result for $n=5$ is just 0.6% above the exact value.

On examining the trends exhibited by the tables, one finds that the effect of increasing n is not only to increase the $\alpha=0$ value of S_n, but also to decrease the large-α values. The increase in the undamped value of S_n is easily understood, since it merely corresponds to an increase in the barrier height. The large-α variation can be established by examining the exactly soluble $n\to\infty$ limit.[2] The $T=0$ action is given by

$$\lim_{n\to\infty}\frac{S_n(\alpha=0)}{(M\omega_0\Delta q^2)}=1 , \tag{10a}$$

while for $\alpha>1$, one has

$$\lim_{n\to\infty}\frac{S_n(\alpha>1)}{(M\omega_0\Delta q^2)}=\frac{\pi\sqrt{\alpha^2-1}}{\ln[(\alpha+\sqrt{\alpha^2-1})/(\alpha-\sqrt{\alpha^2-1})]} . \tag{10b}$$

Thus one sees that the large α behavior of S_n is, in fact, logarithmically suppressed when compared to the $n=1$ case.

After having established the degree of reliability of the variational ansatz, we shall next consider the case of frequency-dependent Ohmic damping.

We shall consider the case in which $k(\tau)$ is given by

$$k(\tau)=\frac{M\eta}{2\pi\tau_0^2}g(\tau/\tau_0) , \tag{11}$$

where $g(x)$ is the auxiliary exponential integral function.[10] This corresponds to Ohmic damping with a Drude

TABLE I. The dimensionless action $S/(M\omega_0\Delta q^2)$ for the potential with $n=1$. The action is given for various values of the damping strengths α and temperatures T/T_0. The results of the variational approximation (VA) are presented alongside the numerical results obtained by Grabert, Olschowski, and Weiss (Ref. 6).

T/T_0	0.1		0.4		0.6		0.8	
α	VA	Ref. 6	VA	Ref. 6	VA	Ref. 6	VA	Ref. 6
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	5.651	5.652	5.368	5.370	4.990	4.993	4.461	4.459
10.00	13.951	13.926	13.251	13.259	12.318	12.296	11.011	11.037

TABLE II. The action S, 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 where $n=3$.

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 action S, in units of $(M\omega_0\Delta q^2)$ calculated for the potential with $n=1$, and the non-Ohmic dissipation given in Eq. (11). We show the results for T/T_0 fixed at 0.1, while the dissipation strength α and the correlation time $\omega_0\tau_0$ are varied.

α \ $\omega_0\tau_0$	0	1	5	10
0.00	0.567	0.567	0.567	0.567
0.05	0.612	0.596	0.581	0.576
0.10	0.659	0.627	0.595	0.584
0.50	1.070	0.899	0.714	0.656
1.00	1.656	1.320	0.886	0.755
2.00	2.942	2.389	1.313	0.984
4.00	5.651	4.978	2.555	1.584
10.00	13.951	13.252	9.972	4.775

cutoff,[11] or to the classical equation of motion

$$M\frac{d^2q}{d\tau^2}+\int_0^{\tau}\frac{M\eta}{\tau_0}\exp\left[-\frac{(\tau-\tau')}{\tau_0}\right]\dot{q}(\tau')d\tau'+\frac{dV(q)}{dq}=0. \tag{12}$$

As τ_0 tends to zero, one recovers the $1/\tau^2$ behavior corresponding to the usual Ohmic damping form of $k(\tau)$. On the other hand, as τ_0 tends to infinity, $k(\tau)$ is suppressed to zero for finite times τ. The effective action is to be evaluated with the same trial function [Eq. (3)], but with $k(\tau)$ given by Eq. (11). Only the dissipative part of S is modified; the term proportional to α in Eq. (5) is replaced by

$$4\alpha\pi y^2\sum_{m=1}^{\infty}\left[\frac{m}{1+m2\pi T\tau_0}\left(\frac{x-1}{x+1}\right)^m\right]. \tag{13}$$

The extremal conditions for the action, $\partial S/\partial x=0$ and $\partial S/\partial y=0$ are reduced to one transcendental equation, which is solved numerically. The results are tabulated in Table IV. We note that, as the correlation time τ_0 increases, the effective action decreases toward its undamped value. Likewise, the temperature T_0 at which the rate crosses over from being dominated by quantum tunneling to that of thermal activation, increases as τ_0 increases.[4] At the crossover temperature the variational approximation becomes exact, and the effective action smoothly matches onto the exponent of the Arrhenius law. All of this is in qualitative agreement with the expectations that, as τ_0 increases, the high-frequency components of the action should increasingly decouple from the heat bath; i.e., the action should tend toward its undamped value.

TABLE III. The variational approximation for the effective action S, calculated with the $n=5$ potential. The action, in units of $(M\omega_0\Delta q^2)$, is shown for various values of the 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

The calculation of the exponential suppression of the decay rate with frequency-dependent damping may be of some importance in the discussion of experiments on rf superconducting quantum interference devices and Josephson junctions,[12–16] since there is experimental evidence[12,14,16] that these systems exhibit these effects.

We have examined the decay from a metastable state using a variational approach. The method has been applied in calculating the dominant exponential part of the rate at low temperatures, where the decay is dominated by quantum tunneling processes. Using a two-parameter trial function we have evaluated the exponent for various potentials and different types of coupling to the thermal reservoir. These results are in excellent agreement with the numerical results for the action calculated by Grabert, Olschowski, and Weiss,[6] as well as those by Chang and Chakravarty[5] for the cubic potential ($n=1$). The accuracy of the variational approximation improves as the potential is varied from $n=1$ to $n=5$. This is verified by comparison to the undamped action. We have also examined the effects of introducing a Drude cutoff in the Ohmic damping process.[11] We see that as the correlation time τ_0 increases, the variational approximation gives results which interpolate between the undamped and Ohmic damping limits.

To summarize, we find that the direct variational approach to the decay rate is an extremely simple one. The method not only reproduces the correct qualitative dependences on the various factors which influence the quantum decay rate, but also gives remarkably good accuracy. Due to the extreme simplicity of the method, it may be of considerable use in the fitting of experimental data,[12–16] as well as estimating the influences of novel damping mechanisms.

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For lack of accuracy in our numerical calculations the precision of our old results for $N \geq 20$ was only 10^{-2}. This problem happened because we used the ground-state function that approximates the energy up to 10^{-7} to evaluate the correlation functions assuming that the error in these functions would be the same. This criterion proves to be correct for $N = 18$ but it is not accurate enough for $N \geq 20$. Now we present the correlation functions with an error of 10^{-6} as was claimed in our paper. The conclusions of our work remain the same.

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Erratum: Decay of a metastable state: A variational approach [Phys. Rev. B 34, 1952 (1986)]

E. Freidkin, Peter Riseborough, and Peter Hanggi

In Eq. (5), the right-hand side should be multiplied by a factor of π. The numerical values, in Tables I through IV, were calculated with the correct formula.