Phenomenological shortcut to dissipative tunneling

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A phenomenological approach to dissipative tunneling, originally put forth by Pollak [Phys. Rev. A **33**, 4244 (1986)], is discussed and contrasted with the bounce formalism. This phenomenological approach is based on the WKB theory for parabolic barrier tunneling. It is quite simple and readily evaluated. We study the results for the leading exponential dissipative decay rate in metastable potentials and contrast them with previous instanton-type (bounce-technique) calculations. In doing so, we compare the zero-temperature decay rate in various metastable potentials, different dissipation mechanisms, and also consider the rate enhancement at very low temperatures. One finds between the two methods unexpected good agreement at weak to moderate dissipation strength; the accuracy decreases with increasing dissipation strength and increasing deviation from a harmonic barrier shape.

I. INTRODUCTION

Tunneling in the presence of dissipation has attracted a great deal of attention in recent years both from a theoretical[1–8] and experimental viewpoint,[9–11] ignited by a flurry of experimental activity for tunneling in Josephson junctions, tunneling microscopy, or resonant tunneling in semiconductors. On the theory side the field did undergo a renaissance, with the work on macroscopic tunneling mainly inspired by the ideas of Caldeira and Leggett.[1] With the present contribution we continue our previous work[7,8] on the quantum decay of a metastable state in the presence of interactions with a thermal reservoir. We shall focus on the dominant exponential dependence of the tunneling rate. Usually the exponential dependence is evaluated by using the bounce solution, i.e., the periodic orbit in complex time describing tunneling under the barrier, which obeys a nonlinear, nonlocal integro-differential equation.[1–5] A somewhat simpler although not as accurate technique relies on a variational approximation.[8] These methods require an appreciable amount of numerical work and thus generally will be invoked only in specific situations where an accurate answer is of interest. Often it becomes necessary to consider a whole series of different barrier forms. In this latter case it would be helpful to have a quick method yielding a qualitatively correct answer. Recently Pollak[12] has proposed such an original method which he termed "sudden-transition-state theory" (sudden TST). Apart from giving a certain amount of direct physical insight into dissipative tunneling, this approach involves a minimum of numerical analysis. In the following we shall compare Pollak's method with results obtained by the bounce method or the variational bounce technique, respectively. In doing so, we shall consider different forms of metastable potentials, finite temperatures, and dissipative mechanisms that exhibit a frequency dependence.

II. POLLAK'S SUDDEN-TST APPROACH VERSUS BOUNCE METHOD

In his approach to dissipative tunneling Pollak[12] was guided by the semiclassical limit of quantum-mechanical transition state theory put forth by Miller.[13,14] In addition, he made use of the harmonic approximation at the barrier top and at the well, respectively. The exponential leading part of the decay rate at temperature $T=0$ is then given by

$$\Gamma \propto \exp\left[\frac{-2\pi E_0}{\hbar\omega_B^*}\right] . \tag{2.1}$$

Hereby ω_B^* denotes the coupling-induced dissipation- and memory-renormalized barrier frequency. It is given by the largest positive root of the relation[15]

$$\omega_B^* = \frac{\omega_B^2}{\omega_B^* + (1/M)\hat{\eta}(\omega_B^*)} , \tag{2.2}$$

with $\omega_B > 0$, denoting the (bare) barrier frequency and $\hat{\eta}(\omega_B^*)$ being the Laplace transform of the memory dissipation $\eta(t-s)$ for a damped particle of mass M moving in the metastable potential $V(x)$, i.e.,

$$M\ddot{x} = -\frac{dV}{dx} - \int_0^t \eta(t-s)\dot{x}(s)ds . \tag{2.3}$$

The effective barrier height is denoted by E_0. For tunneling from the ground state it is given by the (bare) barrier height V_0 and the differences in zero-point energies of all normal modes at the barrier top (λ_i^*) and at the well (λ_i), respectively, i.e.,

$$E_0 = V_0 - \tfrac{1}{2}\hbar\lambda_0 + \tfrac{1}{2}\hbar\sum_i (\lambda_i^* - \lambda_i) . \tag{2.4}$$

Next we compare (2.1) with the exponential leading part as obtained within the bounce technique.[1–8] At temperature $T=0$, the tunneling path (bounce) enters the metastable well at energy $E=0$, i.e., it does not start from the true quantum-mechanical ground state $E = \sum_i \hbar\lambda_i/2$, with ($\lambda_i$) being the coupling-induced normal-mode frequencies at the well. As demonstrated by Miller in Ref. 14, this difference between WKB theory and bounce technique induces within the bounce method a logarithmic correction which is transferred to a prefactor correction proportional to $\hbar^{-1/2}$. Thus the result within the bounce method

$$\Gamma \propto \exp\left[\frac{-S_B}{\hbar}\right], \tag{2.5}$$

with S_B denoting the bounce action, should be compared to Eq. (2.1) only after having substituted E_0 [see Eq. (2.4)] by V_0. Next we define the dimensionless, relative bounce action Δb

$$\Delta b = \frac{S_B(\hat{\eta}) - S_B(\hat{\eta}=0)}{M\omega_0(\Delta q)^2}, \tag{2.6}$$

with Δq being the undamped tunneling distance $V(q_0)=V(q_0+\Delta q)=0$. We shall compare in the following the quantity Δb with the corresponding quantity Δb^{PA} obtained from the Pollak method, i.e.,

$$\Delta b^{\mathrm{PA}} \equiv \frac{2\pi V_0}{M\omega_0(\Delta q_h^2)}\left[\frac{1}{\omega_B^*} - \frac{1}{\omega_B}\right]. \tag{2.7}$$

Here the harmonic tunneling length Δq_h is defined by

$$V_0 \equiv \tfrac{1}{2}M\omega_B^2\left[\frac{\Delta q_h}{2}\right]^2. \tag{2.8}$$

For the metastable potentials under investigation, i.e.,

$$V(q) = \tfrac{1}{2}M\omega_0^2 q^2\left[1 - \left[\frac{q}{\Delta q}\right]^n\right] \tag{2.9}$$

($n=1,3,5,\ldots$), one finds

$$\omega_B = \sqrt{n}\,\omega_0\,,$$
$$V_0 = \tfrac{1}{4}Mn\omega_0^2(\Delta q)^2\left[\frac{2}{n+2}\right]^{(n+2)/n}, \tag{2.10}$$
$$\Delta q = \frac{\Delta q_h}{\sqrt{2}}\left[\frac{n+2}{2}\right]^{(n+2)/2n}$$

We shall see that the dimensionless quantity Δb in (2.6) compares favorably with Δb^{PA}, as defined in (2.7). This allows for a fast method to yield accurate estimates for the relative bounce action $S_B(\hat{\eta}) - S_B(\hat{\eta}=0)$. The whole procedure may be summarized as follows:

(i) First evaluate via (2.2) the classical dissipation renormalized frequency ω_B^*.

(ii) Δb^{PA} is then readily given by (2.7). This is then multiplied by $M\omega_0(\Delta q)^2$ to give a useful and quick expression for the actual difference $S_B(\hat{\eta}) - S_B(\hat{\eta}=0)$.

A. Ohmic damping

Ohmic damping is modeled by a memory-free disspation $\eta(t)$ of the form [see Eq. (2.3)]

$$\eta(t-s) = 2\eta\delta(t-s)\,. \tag{2.11}$$

On the other hand, the properties of the oscillator bath leading to a certain type of dissipation are contained in the spectral density $J(\omega)$ defined as

$$J(\omega) = \frac{\pi}{2}\sum_i \frac{C_i^2}{m_i\omega_i}\delta(\omega-\omega_i)\,, \tag{2.12}$$

where m_i and ω_i are the mass and frequency, respectively, of the ith oscillator, and C_i is its coupling strength to the system. It has been shown,[1] that Ohmic dissipation corresponds to a spectral density of the form

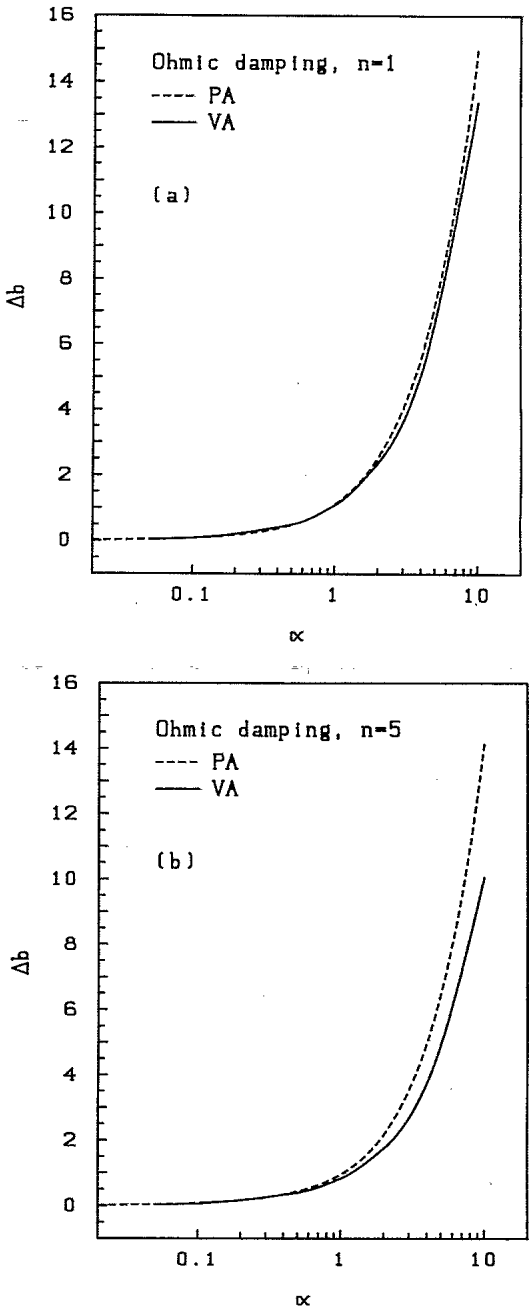

FIG. 1. The exponential part $\Delta b = [S_B(\hat{\eta}) - S_B(\hat{\eta}=0)]/[M\omega_0(\Delta q)^2]$ of the quantum decay rate $\Gamma \propto \exp(-S_B/\hbar)$ at zero temperature and Ohmic dissipation [see Eq. (2.11)] for a cubic potential [$n=1$, Fig. 1(a)] and a metastable potential of higher degree [$n=5$, Fig. 1(b), see Eq. (2.9)], plotted vs the dimensionless damping constant $\alpha \equiv \eta/(2M\omega_0)$, [$\hat{\eta}$ is the Laplace transform of the classical damping function $\eta(t)$]. The solid line corresponds to results of the variational approach (VA, Ref. 8) and the dashed line represents the findings according to Pollak's approach [PA, see Eq. (2.7)].

$$J(\omega)=\eta\omega\Theta(\omega)\ , \tag{2.13}$$

where $\Theta(\omega)$ denotes the unit step function. Using the dissipation given by (2.11) one finds with $\hat{\eta}=\eta$ from (2.2)

$$\omega_B^*=\omega_0[(n+\alpha^2)^{1/2}-\alpha]\ , \tag{2.14}$$

where $\alpha=\eta/(2M\omega_0)$ is the dimensionless damping constant. Replacing V_0 in Eq. (2.7) by Eq. (2.8) we obtain with ω_B^* in Eq. (2.14)

$$\Delta b^{\mathrm{PA}}=\frac{\pi}{4}\left[\frac{n}{(n+\alpha^2)^{1/2}-\alpha}-\sqrt{n}\right]\ . \tag{2.15}$$

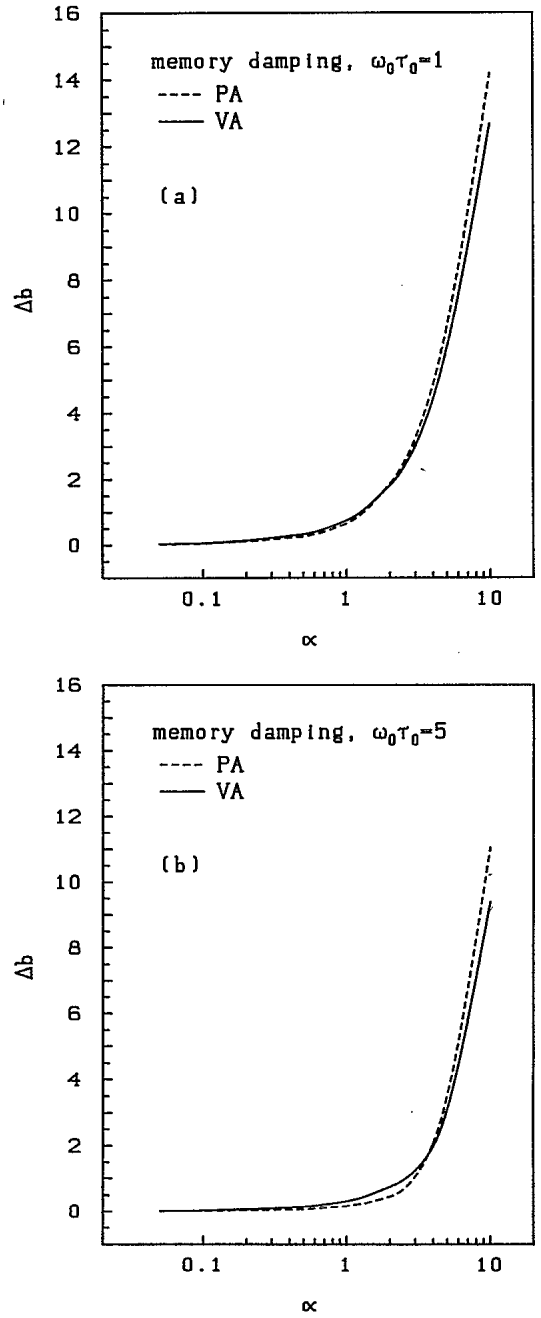

FIG. 2. The exponential part $\Delta b=[S_B(\hat{\eta})-S_B(\hat{\eta}=0)]/[M\omega_0(\Delta q)^2]$ of the quantum decay rate $\Gamma\propto\exp(-S_B/\hbar)$ at zero temperature and memory damping [see Eq. (2.16)] with a correlation time $\omega_0\tau_0=1$ [Fig. 2(a)] and $\omega_0\tau_0=5$ [Fig. 2(b)] for a cubic potential [$n=1$, see Eq. (2.9)], plotted vs the dimensionless damping constant $\alpha\equiv\eta/(2M\omega_0)$, [$\hat{\eta}$ is the Laplace transform of the classical damping function $\eta(t)$]. The solid line corresponds to results of the variational approach (VA, Ref. 8) and the dashed line represents the findings according to Pollak's approach [PA, see Eq. (2.19)].

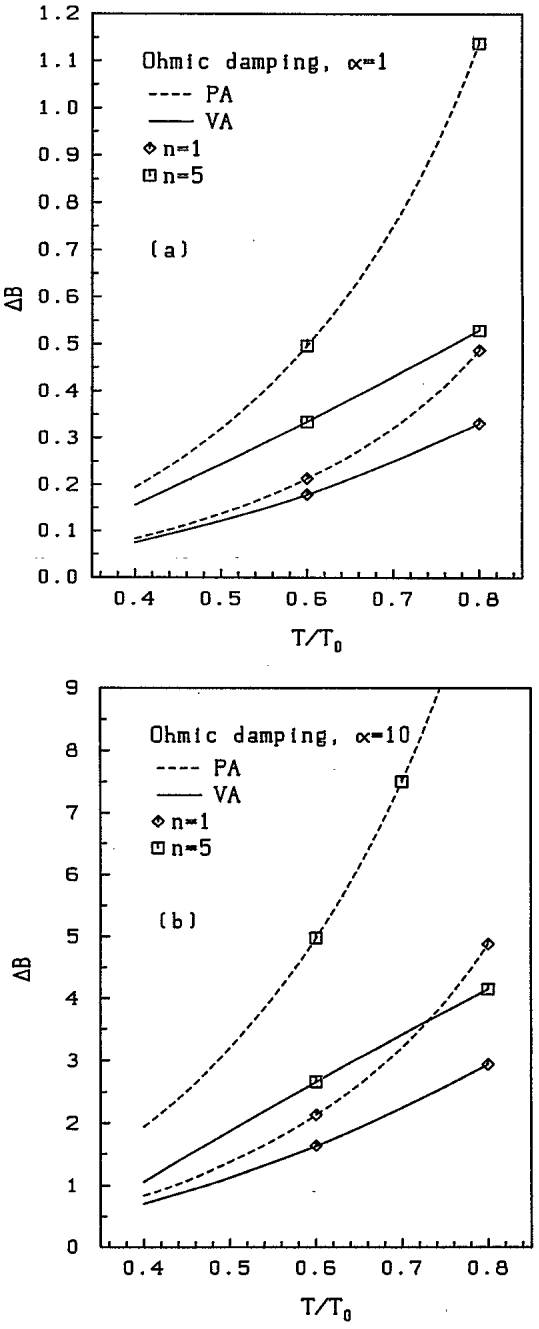

FIG. 3. The thermal enhancement $\Delta B=[S(T)-S(T=0)]/[M\omega_0(\Delta q)^2]$ of the dissipative quantum decay rate $\Gamma\propto\exp(S/\hbar)$ in the case of Ohmic friction [see Eq. (2.11)] with damping strength [$\alpha\equiv\eta/(2M\omega_0)$] $\alpha=1$ [Fig. 3(a)] and $\alpha=10$ [Fig. 3(b)] vs the dimensionless temperature T/T_0 for a cubic potential ($n=1$) and a metastable potential with $n=5$ [see Eq. (2.9)]. The solid line shows the results of the variational approach (VA, Ref. 8) and the dashed line exhibits the findings according to Eq. (2.27) (PA).

In Figs. 1(a) and 1(b) we compare Δb^{PA} as given by (2.15) with results found by using the variational approach of Ref. 8. For the cubic potential [see Fig. 1(a)] the agreement between the two different approaches is excellent. Pollak's approach also agrees quite well with the results of the variational approach for a metastable potential (2.9) with $n=5$ [see Fig. 1(b)]. However, at moderate to strong damping ($1<\alpha<10$) Pollak's results deviate from the variational approach more strongly as compared to the case of the cubic potential. We attribute this behavior to the poorness of approximating the barrier by an inverted parabola. Nevertheless, the overall accuracy in both cases ($n=1$ and 5) is remarkably good.

B. Memory damping

If the bath does not lose its memory instantaneously (Ohmic damping), but has a finite correlation time τ_0 (this means that an action of the system causes a reaction of the bath with an effective duration τ_0), the resulting effect on the coupled system is termed memory friction. A typical representative of such a memory dissipation is the Drude form

$$\eta(t)=\frac{\eta}{\tau_0}\exp(-t/\tau_0)\ . \tag{2.16}$$

The corresponding spectral density of the bath reads

$$J(\omega)=\frac{\eta\omega}{1+\omega^2\tau_0^2}\Theta(\omega)\ . \tag{2.17}$$

Letting $\tau_0\to 0$ in Eq. (2.16) we recover the Ohmic damping case. Calculating ω_B according to Eq. (2.2) with $\eta(t)$ given by (2.16), one finds that ω_B^* is given by the largest, real positive root of the cubic equation

$$\left[\frac{\omega_B^*}{\omega_0}\right]^3\omega_0\tau_0+\left[\frac{\omega_B^*}{\omega_0}\right]^2+\left[\frac{\omega_B^*}{\omega_0}\right](2\alpha-n\omega_0\tau_0)-n=0\ , \tag{2.18}$$

which may be solved numerically. Finally Eq. (2.7) yields

$$\Delta b^{\mathrm{PA}}=\frac{\pi}{4}\left[\frac{n\omega_0}{\omega_B^*}-\sqrt{n}\right]\ . \tag{2.19}$$

Figures 2(a) and 2(b) exhibit Pollak's results for a cubic potential ($n=1$), i.e., Δb^{PA} given by (2.19), together with the corresponding quantity found via the variational approach.[8] Figure 2(a) refers to the dimensionless correlation time $\omega_0\tau_0=1$, whereas Fig. 2(b) displays the results for $\omega_0\tau_0=5$. As in the case of Ohmic damping, we find good agreement between the two different approaches.

C. Tunneling at low temperature

To obtain the thermal rate at low temperatures, Pollak[12] did consider the rate from the ground bath state and the first excited state, in which one bath state is excited while the others remain in the ground state. Up to first order in the squared coupling constants $O(C^2)$, he finds ($\beta=1/k_BT$) for Ohmic damping [see (2.13)]

$$\Gamma(T)=\Gamma(T=0)\exp\left[\frac{\Delta S(T)}{\hbar}\right]\ , \tag{2.20}$$

with

$$\Delta S=\frac{-2\hbar}{\omega_B^* M}\eta\int_0^\infty d\omega\frac{\omega e^{-\beta\hbar\omega}}{\omega^2+\omega_B^2}+\frac{4V_0}{\pi\hbar\omega_0^2 M}\frac{n+2}{n}\eta\int_0^\infty d\omega\frac{e^{-\beta\hbar\omega}}{\omega}\left[\cosh\left[\frac{2\pi\omega}{\omega_B^*}\right]-1\right] \tag{2.21}$$

and ω_B^* is given by Eq. (2.14). For $T<T_0$ Eq. (2.21) can be integrated to give $\{\Delta B^{\mathrm{PA}}\equiv\Delta S(T)/[M\omega_0(\Delta q_h)^2]\}$

$$\Delta B^{\mathrm{PA}}=-\alpha\left[\frac{n+2}{2\pi}\ln\left[1-\frac{T^2}{T_0^2}\right]+\frac{\hbar\omega_0}{2V_0}\frac{n}{(n+\alpha^2)^{1/2}-\alpha}g\left[\frac{T_0}{T}\frac{2\pi n^{1/2}}{(n+\alpha^2)^{1/2}-\alpha}\right]\right]\ , \tag{2.22}$$

where $g(x)$ is the auxiliary sine-cosine integral function[16] and $T_0=\hbar\omega_0[(n+\alpha^2)^{1/2}-\alpha]/(2\pi k_B)$ is the crossover temperature to activated thermal hopping.[3,6,17] The second contribution is proportional to $\hbar\omega_0/(2V_0)$ and thus quite small if compared with the leading first contribution. The $[\hbar\omega_0/(2V_0)]$ contribution yields within the bounce formulation a very small negative temperature correction to the prefactor and should, just as before, be neglected if compared with the temperature dependence of the bounce action.[3] Upon expanding the logarithm in (2.22), we find a thermal enhancement proportional to T^2, i.e.,

$$\Delta B^{\mathrm{PA}}=\alpha\frac{n+2}{2\pi}\frac{T^2}{T_0^2}\ , \tag{2.23}$$

which is in accordance with the findings in Ref. 3.

It is interesting to compare the proportionality factors of the T^2 law of Eq. (2.23) with the universal T^2 law found in Ref. 3 given by

$$\Delta B=\frac{\pi\alpha}{3}\left[\frac{k_BT\tau_B}{\hbar}\right]^2\ , \tag{2.24}$$

where τ_B is the bounce length. For the cubic potential ($n=1$), τ_B was deduced in Ref. 18,

$$\tau_B = \frac{12}{\pi\omega_0} \frac{1}{[\alpha^2+(3/\pi)^2]^{1/2}-\alpha} . \quad (2.25)$$

Inserting τ_B one finds for ΔB

$$\Delta B = \alpha \frac{3}{2\pi} \frac{T^2}{T_0^2} \frac{8}{\pi^2} \frac{[(\alpha^2+1)^{1/2}-\alpha]^2}{\{[\alpha^2+(3/\pi)^2]^{1/2}-\alpha\}^2} . \quad (2.26)$$

Assuming that $3/\pi \sim 1$, we note that (2.26) underestimates (2.23) by the factor of $8/\pi^2 \approx 0.81$ which shows that (2.23) is a fairly good approximation to the T^2 law found by instanton methods.

In Figs. 3(a) and 3(b) we compare the logarithmic (Pollak) approximation

$$\Delta B^{\mathrm{PA}} = -\alpha \frac{n+2}{2\pi} \ln\left[1-\frac{T^2}{T_0^2}\right] \quad (2.27)$$

(valid for $T < T_0$) with the variational results obtained in Ref. 8 both for $\alpha = 1$ [Fig. 3(a)] and large damping $\alpha = 10$ [Fig. 3(b)]. First let us consider the cubic potential ($n=1$). At low to moderate damping $\alpha \sim 1$, one finds surprisingly good agreement with the variational results up to $T/T_0 < 0.5$ which in turn coincides with the numerical results of Ref. 19 within $\lesssim 4\%$. For larger dissipation strength the agreement becomes less satisfactory, although the qualitative trends are still retained. For the metastable potential with $n=5$, the qualitative trends are still reproduced correctly, although the overall accuracy decreases with increasing n.

III. CONCLUSIONS

In this paper we have exploited Pollak's ideas[12] in order to generate a direct and simple estimate for the leading part of the dissipative decay rate from a metastable state. For low to moderate damping, $\alpha < 1$, the agreement between the simple estimate controlled by the dissipation-renormalized barrier frequency ω_B^* in Eqs. (2.14), (2.15), and (2.19) and the variational results[8] is surprisingly good. Admittedly, the estimate decreases in accuracy with increasing n (i.e., increasing deviation from a harmonic barrier shape) and increasing dissipation strength. Most surprising was the qualitative agreement of the temperature dependence at weak to moderate dissipation strength with the simple logarithmic estimate

$$\Delta B^{\mathrm{PA}} = -(\alpha/2\pi)(n+2)\ln(1-T^2/T_0^2) .$$

Having made a comparison for different potentials and damping mechanisms, the simple estimates in (2.15) and (2.19), and (2.27) should prove to be quite useful in obtaining qualitative results and descriptions for various experimental situations or realistic complex memory frictions.[11,20] We hope that these simple estimates find their way into the planning stage of new experiments and effects.

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