Activated decay rate: Finite-barrier corrections

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The activated escape of an underdamped Brownian particle out of a deep potential well is characterized by weak friction $\gamma \ll \omega$ (γ is the coefficient of friction and ω is a typical frequency of the intrawell motion) and by a large barrier height $U_0 \gg T$ (U_0 is the barrier height and T is the temperature). The approach developed previously to calculate the decay rate is based on the derivation of an integral equation and enables one to sum up an infinite series in powers of the ratio $\gamma U_0/T\omega \sim 1$ contributing to the preexponential factor of the Arrhenius law. In the present paper it is shown that the leading correction to the above result comes from the slowing down of the particle motion near the top of the barrier and is of the order of $(T/U_0)\ln(U_0/T)$. To calculate it explicitly, one needs to find a correction to the kernel of the above-mentioned integral equation. Beyond the leading-logarithmic approximation, two different factors contribute corrections of the order of $T/U_0 \sim \gamma/\omega$. The noise-induced effects in the barrier crossing-recrossing by particles in a narrow energy range $\varepsilon \sim \gamma T/\omega$ can be easily incorporated into the general scheme of the calculations. On the other hand, a more accurate derivation of the kernel of the integral equation is required to take into account small variations of the intrawell particle motion caused by variations of the particle energy on the scale $T \ll U_0$ under the effects of friction and thermal noise. The proposed consistent expansion in terms of the small parameters of the problem provides an effective approach to a quantitative investigation of the turnover behavior in the Kramers problem. For the regime of an intermediate-to-strong friction, the finite-barrier corrections can be neglected, since, for typical barrier shapes, they are always small.

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I. INTRODUCTION

The activated decay of metastable states is a common feature of many physical and chemical systems. These systems are characterized by a number of nearly stable states separated by high potential barriers. Transitions between different potential minima due to the thermal fluctuations are exponentially rare if the barrier height U_0 is large compared to the temperature T. In this limit the decay rate (inverse lifetime) of the metastable state is described by the Arrhenius law

$$\frac{1}{\tau}=\frac{\Omega}{2\pi}A\exp\left[-\frac{U_0}{T}\right], \tag{1}$$

where Ω is the frequency of small oscillations near the bottom of the potential well. Other details of the internal structure of the system and of its interaction with the environment are absorbed into the preexponential factor A. The condition of metastability, $\tau\Omega \gg 1$, requires $U_0 \gg T$. However, the exponential dependence of τ on the barrier height provides a long lifetime even for a moderate ratio $U_0/T > 5$. With a further increase of this ratio, the decay events become too rare to be observable. Hence, one arrives at the conclusion that the ratio U_0/T must be considered as large in its quality of the argument of the exponential. At the same time, corrections in the inverse parameter, T/U_0, may still be of some importance when calculating the preexponential factor A. This general observation can be clarified by considering the escape of a Brownian particle out of a one-dimensional potential well. Originally, this model was proposed by Kramers in order to elucidate the process of thermal dissociation of a molecule interacting with a gas of light particles [1]. Many decades later it was realized that a resistively shunted Josephson junction represents virtually the only experimental system embodying all the features of the Kramers theoretical model [2]. An exhaustive survey of the issues related to the Kramers problem can be found in a review article [3]. A detailed exposition of the mathematical methods and physical results for an underdamped Brownian motion in deep potential barriers is given in Ref. 4. Since the physical aspects of the problem are discussed already in the above-mentioned articles and reviews, it is worthwhile to focus mostly on mathematical procedures.

The starting point is the Fokker-Planck equation,

$$\frac{p}{m}\frac{\partial f}{\partial x}-\frac{dU(x)}{dx}\frac{\partial f}{\partial p}=\gamma\frac{\partial}{\partial p}\left[mT\frac{\partial f}{\partial p}+pf\right], \tag{2}$$

for the distribution function $f(p,x)$ of a Brownian particle with the mass m, coordinate x, and momentum p moving in the potential $U(x)$ with the friction coefficient γ. The function $f(p,x)$ is assumed to be normalized to one particle in the potential well,

$$\int f(p,x)dp\,dx=1\ . \tag{3}$$

Near the bottom of the well, the distribution function is close to the equilibrium one,

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$$f(p,x)\approx\frac{\Omega}{2\pi T}\exp\left[-\frac{p^2}{2mT}-\frac{U(x)-U_0}{T}\right], \quad (4)$$

where Ω is the frequency of small oscillations near the bottom of the well and U_0 is the height of the barrier. For definiteness, the top of the barrier is placed at $x=0$ and is described by the asymptotics

$$U(x)\approx-\tfrac{1}{2}m\omega^2x^2 . \quad (5)$$

At the outside of the barrier there are no particles, with exception of those escaping out of the well, which yield the boundary condition

$$f(p,x)\to 0; \quad x\to\infty . \quad (6)$$

The decay rate is given by the flux of the particles across the top of the barrier,

$$\frac{1}{\tau}=\int_{-\infty}^{\infty}f(p,0)\frac{p}{m}dp . \quad (7)$$

Substitution into this expression of the Boltzmann distribution and integration over positive momenta yields Eq. (1) with the preexponential factor $A=1$. In the major part of this paper, the underdamped escape will be considered. Then, at energies close to the top of the barrier, the distribution is depleted due to the escape of particles across the barrier, since the excitation of particles by thermal noise is too weak to reestablish the equilibrium shape of the distribution function. In this case the preexponential factor A is smaller than unity and depends on the noise strength, temperature, etc.

It should be noted that in an underdamped case, when the coefficient of friction is small,

$$\gamma\ll\Omega,\omega , \quad (8)$$

the entire energy of a particle,

$$\varepsilon\equiv\frac{p^2}{2m}+U(x) , \quad (9)$$

is nearly conserved in one cycle of its motion in the well. This justifies working out a perturbational approach starting from the particle trajectory at a given energy ε in the absence of friction and noise. Then, from a formal point of view, the preexponential factor A can be thought of as a function of the two dimensionless parameters, γ/ω and T/U_0. In a leading approximation, the expansion of A in the small parameter γ/ω has the following form [5]:

$$A_0=\sum_{n=0}^{\infty}a_n(\gamma U_0/\omega T)^{1+n/2} . \quad (10)$$

This series has a finite radius of convergence. However, as an analytical function it makes sense for any value of its argument,

$$\Delta\equiv\frac{\delta}{T}\sim\frac{\gamma U_0}{\omega T} , \quad (11)$$

where $\delta\sim\gamma U_0/\omega$ is the energy loss per one cycle of motion at the barrier height. For the function $A_0(\Delta)$, the following integral representation was obtained [5]:

$$A_0(\Delta)=\exp\left\{\frac{1}{\pi}\int_0^{\infty}\frac{\ln\{1-\exp[-\Delta(\lambda^2+\frac{1}{4})]\}d\lambda}{\lambda^2+\frac{1}{4}}\right\} . \quad (12)$$

Asymptotically, this yields

$$A_0(\Delta)\approx\Delta+\zeta(\tfrac{1}{2})\Delta^{3/2}/\pi^{1/2}\approx\Delta-0.82\Delta^{3/2}; \quad \Delta\ll 1 , \quad (13)$$

where $\zeta(x)$ is the Rieman ζ function, and

$$A_0(\Delta)\approx 1-2(\pi\Delta)^{-1/2}\exp(-\Delta/4), \quad \Delta\gg 1 . \quad (14)$$

A naive guess is that corrections to this result must be expandable in powers of the small parameters T/U_0 and γ/ω. It will be shown, however, that, due to the slowing down of the particle motion near the barrier top, the perturbative expansion for A looks rather like

$$A(\gamma/\omega,T/U_0)\approx A_0(\Delta)-\frac{T}{U_0}\frac{U_0}{\omega S}\left[A_1(\Delta)\ln\frac{U_0}{T}+B_1(\Delta)\right], \quad (15)$$

where S is the action per cycle of motion of an escaping particle (an explicit expression for S is given below), the dependence on the ratio $\gamma U_0/\omega T$ is displayed through the positive functions $A_1(\Delta)$ and $B_1(\Delta)$ of the argument

$$\Delta\equiv\frac{\gamma S}{T}=\frac{U_0}{T}\frac{\gamma}{\omega}\frac{\omega S}{U_0} , \quad (16)$$

and the ratio $\omega S/U_0$ is a dimensionless number determined by the shape of the potential $U_0(x)$.

The general frame of this paper is as follows. In Sec. II, the energy-diffusion equation is solved and the general structure of an asymptotic expansion of $A(\gamma/\omega,T/U_0)$ in the limit of small Δ, when $\gamma/\omega\ll T/U_0$, is discussed. In Sec. III, the opposite limit, $1\gg\gamma/\omega\gg T/U_0$, is considered. Then, the flux of escaping particles is Boltzmannian with an exception of a narrow range of energies, $\varepsilon\sim\gamma T/\omega\ll T$, where under effects of the thermal noise the distribution function acquires a fine structure. This results in a relative suppression of the decay rate in proportion to the small parameter $\gamma/\omega\ll 1$. In Sec. IV, a general scheme of the integral equation approach is exposed and the explicit expression (12) for $A_0(\Delta)$ is derived. In Sec. V, the kernel of the integral equation is calculated to leading order in $(T/U_0)\ln(U_0/T)$, when the main contribution is due to the slowing down of the particle motion near the barrier top. In Sec. VI, the corrected kernel is solved and an expression for the function $A_1(\Delta)$ is derived. In Sec. VII, a contribution to the function $B_1(\Delta)$ from the noise-induced reflections and the barrier recrossings is calculated. In Sec. VIII, the kernel of the integral equation is calculated beyond the leading-logarithmic correction and in Sec. IX, a complete expression for the function $B_1(\Delta)$ is found. In Sec. X, the results obtained are applied to a quantitative analysis of the turnover problem for the preexponential factor

$A(\gamma/\omega, T/U_0)$. Section XI considers linear corrections in T/U_0 in the regime of an intermediate-to-strong friction.

II. ENERGY-DIFFUSION REGIME

To consider the limit $\gamma \to 0$, Eq. (2) must be transformed to the energy variable,

$$\frac{\partial f}{\partial x} = \pm\gamma \frac{\partial}{\partial \varepsilon} p(\varepsilon, x) \left[T\frac{\partial f}{\partial \varepsilon} + f \right] , \tag{17}$$

where

$$p(\varepsilon, x) \equiv \{2m[\varepsilon - U(x)]\}^{1/2} \tag{18}$$

is the absolute value of the momentum for a particle with an energy ε at a point x and the signs $\pm$ denote the direction of motion. Averaging Eq. (17) over x at a given energy yields the energy-diffusion equation [1],

$$\frac{\partial}{\partial \varepsilon} \delta(\varepsilon) \left[T\frac{\partial f}{\partial \varepsilon} + f \right] = 0 , \tag{19}$$

where the diffusion coefficient $\delta(\varepsilon)$ is given by

$$\delta(\varepsilon) = \gamma S(\varepsilon) = 2\gamma \int_{x_1}^{x_2} \{2m[\varepsilon - U(x)]\}^{1/2} dx . \tag{20}$$

The points $x_{1,2}(\varepsilon)$ are the turning points,

$$U(x_{1,2}) = \varepsilon , \tag{21}$$

and the function $S(\varepsilon)$ is the action per cycle. The solution of Eq. (19) with the boundary condition

$$f(0) = 0 \tag{22}$$

is given by

$$f(\varepsilon) = \frac{\Omega}{2\pi T} \exp\left[-\frac{\varepsilon + U_0}{T} \right] \times \int_{\varepsilon}^{0} \frac{\exp(\varepsilon/T) d\varepsilon}{\delta(\varepsilon)} \left[\int_0^{\infty} \frac{\exp(-\varepsilon'/T)}{\delta(-\varepsilon')} d\varepsilon' \right]^{-1} . \tag{23}$$

A correction from the energy dependence of Ω near the bottom of the potential well is neglected, as our principal aim here is the calculation of a leading correction to A coming from $\delta(\varepsilon)$. The relation

$$\frac{1}{\tau} = -\delta(\varepsilon) T \frac{df(\varepsilon)}{d\varepsilon} \bigg|_{\varepsilon=0} \tag{24}$$

which can be derived with the use of Eqs. (2) and (22) (see also Ref. [1]), yields

$$\frac{1}{\tau} = \frac{\Omega}{2\pi} \exp\left[-\frac{U_0}{T} \right] \left[\int_0^{\infty} \frac{\exp(-\varepsilon/T) d\varepsilon}{\delta(-\varepsilon)} \right]^{-1} . \tag{25}$$

The function $\delta(\varepsilon)$ can be expanded in an asymptotic series in ε. For our purposes, the first-order correction has to be considered,

$$\delta(\varepsilon) \approx \delta + \frac{\gamma}{\omega} \varepsilon \left[\ln\frac{U_0}{T} + C_U + 1 + \ln 2 - \ln\frac{|\varepsilon|}{T} \right] , \tag{26}$$

where

$$\delta \equiv \delta(0) \equiv \gamma S , \tag{27}$$

S is the action per cycle of motion with $\varepsilon = 0$,

$$S = 2\int_{x_1}^{0} [-2mU(x)]^{1/2} dx , \tag{28}$$

and C_U is a number dependent on the shape of the potential $U(x)$,

$$C_U \equiv 2\int_{x_1}^{0} dx \left\{ \frac{m\omega}{[-2mU(x)]^{1/2}} + \frac{1}{x} \right\} + \ln\frac{m\omega^2 x_1^2}{U_0} . \tag{29}$$

Physically, δ is the energy loss per cycle of motion calculated in a linear approximation in γ,

$$\delta \equiv \gamma m \oint \left[\frac{dx}{dt} \right]^2 dt , \tag{30}$$

where $dx(t)/dt$ is the solution of the Newton equation in the potential $U(x)$ with the entire energy $\varepsilon = 0$. Substitution of Eq. (26) into Eq. (25) and expansion in the small parameter γ/ω then yields

$$A(\gamma/\omega, T/U_0) \approx \Delta - \frac{T}{U_0}\frac{U_0}{\omega S} \left[\Delta \ln\frac{U_0}{T} + \Delta(C_U + 2 + \ln 2 - C) \right] , \tag{31}$$

where $C \simeq 200.5772$ is the Euler number. Comparing this expression with the definition (15) yields the asymptotics

$$A_0(\Delta) \approx \Delta; \quad \Delta \ll 1 \tag{32}$$

$$A_1(\Delta) \approx \Delta; \quad \Delta \ll 1 \tag{33}$$

$$B_1(\Delta) \approx \Delta(C_U + 2 + \ln 2 - C); \quad \Delta \ll 1 . \tag{34}$$

On this stage, all the parameters of the problem are introduced. We have calculated them for two typical potentials. For a cubic potential

$$U(x) = -\frac{m\omega^2 x^2}{2} \left[1 - \frac{x}{x_1} \right] , \tag{35}$$

one obtains

$$\frac{U_0}{\omega S} = \frac{5}{36} \approx 0.1389 ; \tag{36}$$

$$C_U = 3\ln 6 \approx 5.375 . \tag{37}$$

For a quartic potential

$$U(x) = -\frac{m\omega^2 x^2}{2} \left[1 - \frac{x^2}{x_1^2} \right] , \tag{38}$$

one obtains

$$\frac{U_0}{\omega S} = \frac{3}{16} \approx 0.1875 ; \tag{39}$$

$$C_U = 5\ln 2 \approx 3.466 . \tag{40}$$

The above results, obtained in a linear-in-γ/ω approximation, reveal a rather complicated structure of the asymptotic expansion for A in the second small parameter T/U_0. With the account of further terms, this expansion takes the form

$$A(\gamma/\omega, T/U_0) \approx \Delta \sum_{n=0}^{\infty} \left[\frac{T}{U_0}\right]^n P_n\left[\ln\frac{U_0}{T}\right]; \quad \gamma/\omega \to 0 \tag{41}$$

where $P_n(x)$ is a polynomial function. In a series of papers a modified expression for A was proposed [6,7]. It exploits essentially Eq. (12) with Δ multiplied by a function of γ/ω [8,9]. Naturally, in the limit of $\gamma/\omega \to 0$ only the first term of Eq. (41) is reproduced.

III. EFFECTS OF RECROSSINGS

If the energy dissipation is sufficiently strong, $\delta \gg T$, particles succeed to be thermalized during their intrawell motion and the flux of the right-going particles near the top of the barrier is nearly Boltzmannian. In this case, solution of the approximate equation near the top of the barrier,

$$\frac{p}{m}\frac{\partial f}{\partial x} + m\omega^2 x \frac{\partial f}{\partial p} = \gamma \frac{\partial}{\partial p}\left[mT\frac{\partial f}{\partial p} + pf\right], \tag{42}$$

in the limit of $\gamma/\omega \ll 1$ is given by [1]

$$f(p,x) = \frac{\Omega}{2\pi T}\exp\left[-\frac{U_0}{T} - \frac{p^2 - m^2\omega^2 x^2}{2mT}\right]\left[\frac{1}{2\pi m\gamma T}\right]^{1/2} \times \int_{-\infty}^{p-m\omega x} \exp\left[-\frac{\omega u^2}{2m\gamma T}\right] du . \tag{43}$$

The flux of escaping particles yields the decay rate

$$\frac{1}{\tau} = \int_{-\infty}^{\infty} \frac{p}{m} f(p,0)\,dp = \frac{\Omega}{2\pi}\left[1 - \frac{\gamma}{2\omega}\right]\exp\left[-\frac{U_0}{T}\right]. \tag{44}$$

Comparing with Eq. (1), one can write

$$A \approx 1 - \frac{\gamma}{2\omega} \equiv 1 - \frac{1}{2}\frac{T}{U_0}\frac{U_0}{\omega S}\Delta, \quad 1 \ll \Delta \ll U_0/T . \tag{45}$$

In turn, comparison with Eq. (15) yields the following asymptotics:

$$A_0(\Delta) \approx 1; \quad \Delta \gg 1 \tag{46}$$

$$A_1(\Delta) \approx 0; \quad \Delta \gg 1 \tag{47}$$

$$B_1(\Delta) \approx \Delta/2; \quad \Delta \gg 1 . \tag{48}$$

In the following sections we will find explicit expressions for $A_0(\Delta)$, $A_1(\Delta)$, and $B_1(\Delta)$ which are applicable for arbitrary Δ and have as its asymptotics Eqs. (32)–(34) for $\Delta \ll 1$ and Eqs. (46)–(48) for $\Delta \gg 1$.

IV. INTEGRAL-EQUATION FORMALISM

To generalize the above results for finite values of $\Delta \equiv \delta/T$, one has to find a perturbative solution of the Fokker-Planck equation (18). In this section, an earlier developed approach to the calculation of $A_0(\Delta)$ is briefly described. Some quantities and concepts introduced in this way will be used for further extension of this approach.

The typical energies of the escaping particles are small compared with the typical potential energy $\varepsilon \sim T \ll U_0$. In neglecting corrections of the order of $T/U_0 \ll 1$, the differential equation (17) is equivalent to the integral equation

$$f(\varepsilon,x) = \int_{-\infty}^{\infty} g(\varepsilon,\varepsilon';x,x') f(\varepsilon',x')\,d\varepsilon' . \tag{49}$$

The Green function $g(\varepsilon,\varepsilon',x,x')$ is governed by the equation

$$\frac{\partial g}{\partial x} = \pm\gamma \frac{\partial}{\partial \varepsilon}[-2mU(x)]^{1/2}\left[T\frac{\partial g}{\partial \varepsilon} + g\right]. \tag{50}$$

The initial condition at the starting point $x = x'$ is

$$g(\varepsilon,\varepsilon';x,x) = \delta_D(\varepsilon - \varepsilon') , \tag{51}$$

where $\delta_D(z)$ is the Dirac σ function. Obviously, the solution of Eq. (50) is a Gaussian function of $\varepsilon - \varepsilon'$. For our purposes we need only the Green function for a basic trajectory, which starts from the barrier top, $x = 0$, goes to the turning point, $x = x_1$, and backwards as

$$g_0(\varepsilon - \varepsilon') = (4\pi\delta T)^{-1/2}\exp\left[-\frac{(\varepsilon - \varepsilon' + \delta)^2}{4\delta T}\right]. \tag{52}$$

The parameter δ is the energy loss per cycle of motion given by Eq. (27). This Green function describes the probability of a particle returning to the barrier with energy ε after a cycle of motion, if its initial energy when reflecting from the barrier was equal to ε'. Near the top of the barrier, the energy distribution function $f(\varepsilon)$ is established by the particles which failed to cross the barrier at the previous attempt because their energies were negative $\varepsilon' < 0$. This simple consideration enables one to write down the integral equation [10]

$$f(\varepsilon) = \int_{-\infty}^{0} g_0(\varepsilon - \varepsilon') f(\varepsilon')\,d\varepsilon' . \tag{53}$$

This equation has to be solved with the boundary condition that, for energies deep in the potential well, $f(\varepsilon)$ is Boltzmannian,

$$f(\varepsilon) \approx \frac{\Omega}{2\pi T}\exp\left[-\frac{\varepsilon + U_0}{T}\right]; \quad |\varepsilon| \gg T; \quad \varepsilon < 0 . \tag{54}$$

The decay rate is then given by the relation

$$\frac{1}{\tau} = \int_0^{\infty} f(\varepsilon)\,d\varepsilon \tag{55}$$

which explicitly neglects contributions from the particles recrossing the barrier.

To solve the integral equation by the Wiener-Hopf method, the one-sided Fourier transformation is introduced,

$$f_{\pm}(\lambda)=\frac{2\pi}{\Omega}\int_{-\infty}^{\infty}\Theta(\pm\varepsilon)\exp\left[\frac{i\lambda\varepsilon}{T}+\frac{\varepsilon}{2T}+\frac{U_0}{T}\right]f(\varepsilon)d\varepsilon\ , \tag{56}$$

where Θ denotes the conventional steplike function. The integral equation takes the form

$$f_+(\lambda)+f_-(\lambda)=g_0(\lambda)f_-(\lambda)\ , \tag{57}$$

where

$$g_0(\lambda)=\exp[-\Delta(\lambda^2+\tfrac{1}{4})] \tag{58}$$

and

$$\Delta\equiv\delta/T\ . \tag{59}$$

After rewriting the equation

$$f_+(\lambda)=-G(\lambda)f_-(\lambda)\ , \tag{60}$$

the function

$$G(\lambda)\equiv 1-g_0(\lambda) \tag{61}$$

must be separated into the factors, analytical in the upper and lower half-planes of complex λ

$$G(\lambda)=G_+(\lambda)G_-(\lambda)\ , \tag{62}$$

where

$$\ln G_{\pm}(\lambda)=\pm\int\frac{d\lambda'}{2\pi i}\frac{\ln G(\lambda')}{\lambda'-\lambda\mp i0}\ . \tag{63}$$

In an extremely underdamped limit one has

$$G_{\pm}(\lambda)=\mp i\Delta^{1/2}(\lambda\pm i/2),\quad \Delta\ll 1\ . \tag{64}$$

Equation (60) can now be written in the form

$$\frac{f_+(\lambda)}{g_+(\lambda)}=-f_-(\lambda)g_-(\lambda)\ . \tag{65}$$

The two sides of this equation are analytical, respectively, in the upper and lower half-planes of λ and have a common stripe of analyticity. This means that they are equal to a simple function of λ which must be found from a boundary condition. In our case, this condition is given by Eq. (54) which after the Fourier transformation (56) yields

$$f_-(\lambda)\approx-\frac{1}{\lambda+i/2};\quad |\lambda+i/2|\ll 1\ . \tag{66}$$

The explicit solutions of Eq. (65) with the boundary condition (66) look like [5]

$$f_+(\lambda)=\frac{iG_+(\lambda)G_-(-i/2)}{\lambda+i/2}\ , \tag{67}$$

$$f_-(\lambda)=-\frac{iG_-(-i/2)}{G_-(\lambda)(\lambda+i/2)}\ . \tag{68}$$

The function $f_+(\lambda)$ is analytical in the entire plane of complex λ since $f(\varepsilon)$, according to Eq. (53), decreases for $\varepsilon\to\infty$ sooner than any exponential function,

$$f(\varepsilon)\sim\exp(-\varepsilon^2/4T\delta),\quad \varepsilon\gg(T\delta)^{1/2}\ . \tag{69}$$

In contrast, $f_-(\lambda)$ is analytical for $\mathrm{Im}\lambda<-\frac{1}{2}$. The preexponential factor is obtained from the relation

$$A_0(\Delta)=f_+(i/2) \tag{70}$$

which reproduces Eq. (12).

V. LEADING-LOGARITHMIC APPROXIMATION

In order to calculate the function $A_1(\Delta)$, one has to solve the equation

$$\frac{\partial f}{\partial x}=\pm\gamma\frac{\partial}{\partial\varepsilon}\{2m[\varepsilon-U(x)]\}^{1/2}\left[T\frac{\partial f}{\partial\varepsilon}+f\right] \tag{71}$$

to leading order in the parameter $T/U_0\ln(U_0/T)$. We resort again to the integral equation

$$f(\varepsilon)=\int_{-\infty}^{0}g(\varepsilon,\varepsilon')f(\varepsilon)d\varepsilon\ , \tag{72}$$

where the Green function $g(\varepsilon,\varepsilon')$ must be obtained via integration of a corrected equation,

$$\frac{\partial g}{\partial x}=\pm\gamma\frac{\partial}{\partial\varepsilon}\{[-2mU(x)]^{1/2}+\varepsilon[-m/2U(x)]^{1/2}\}\times\left[T\frac{\partial g}{\partial\varepsilon}+g\right]\ , \tag{73}$$

along the basic trajectory.

To solve the equation for $g(\varepsilon,\varepsilon',x)$, it is convenient to introduce the new function,

$$g(\lambda,\varepsilon',x)\equiv\int g(\varepsilon,\varepsilon',x)\exp\left[\frac{i\lambda(\varepsilon-\varepsilon')}{T}+\frac{\varepsilon-\varepsilon'}{2T}\right]d\varepsilon\ , \tag{74}$$

which obeys the equation

$$\frac{\partial g(\lambda,\varepsilon',x)}{\partial x}=\pm\frac{\gamma}{T}[-2mU(x)]^{1/2}(\lambda^2+\tfrac{1}{4})g(\lambda,\varepsilon',x)\ ,$$
$$\pm\gamma[-m/2U(x)]^{1/2}\left[\lambda-\frac{i}{2}\right]\left[-i\frac{\partial}{\partial\lambda}+\frac{\varepsilon'}{T}\right]\times\left[\lambda+\frac{i}{2}\right]g(\lambda,\varepsilon',x)\ , \tag{75}$$

with the initial condition

$$g(\lambda,\varepsilon',\tilde{x})=1\ . \tag{76}$$

We have introduced here a coordinate $\tilde{x}$ which will be used later as a cutoff parameter. After the substitution

$$g=g_0[1+g_1];\quad g_1\ll 1\ , \tag{77}$$

one obtains the simple equation

$$\frac{\partial g_1(\lambda,\varepsilon',x)}{\partial x}=\pm\gamma[-m/2U(x)]^{1/2}\times\left[(\lambda^2+\tfrac{1}{4})\frac{\varepsilon'+2i\delta(x)}{T}-i\lambda-\frac{1}{2}\right], \tag{78}$$

where $\delta(x)$ is the magnitude or the energy dissipation for the particle motion along the basic trajectory from point $\tilde{x}$ to point x. To calculate $g_1(\lambda,\varepsilon)$, one has to integrate the right-hand side of Eq. (78) from $\tilde{x}$ to the left-hand turning point x_1 and back. This integral is logarithmically divergent,

$$\int_{x_1}^{\tilde{x}}\left[-\frac{m}{2U(x)}\right]^{1/2}dx\approx\ln\frac{x_1}{\tilde{x}},\quad |\tilde{x}|\ll|x_1|\ . \tag{79}$$

In the leading-logarithmic (LL) approximation, we are not interested in a numeric factor under the sign of logarithm, so that this result must be substituted by $(\frac{1}{2})\ln(U_0/T)$. For the term containing the function $\delta(x)$, the final part of the trajectory only contributes to a logarithmic divergency, where $\delta(x)$ has to be substituted by $\delta\equiv T\Delta$. The result of these calculations is given by

$$g_1^{\rm LL}(\lambda,\varepsilon')=-\frac{\gamma}{\omega}\ln\frac{U_0}{T}\left[(\lambda^2+\tfrac{1}{4})\left[\frac{\varepsilon'}{T}+i\Delta\lambda\right]-i\lambda-\frac{1}{2}\right]. \tag{80}$$

The inverse Fourier transformation then yields

$$g_1^{\rm LL}(\varepsilon,\varepsilon')=-\frac{\gamma}{\omega}\ln\frac{U_0}{T}\left\{(\varepsilon+\varepsilon')\left[\frac{1}{8}+\frac{1}{4\Delta}-\frac{(\varepsilon-\varepsilon')^2}{8\Delta^2T^2}\right]-\frac{1}{2}\right\}. \tag{81}$$

VI. SOLUTION OF THE CORRECTED INTEGRAL EQUATION

The corrected integral equation in the Fourier representation looks like

$$f_+(\lambda)+G(\lambda)f_-(\lambda)=g_0(\lambda)\int_{-\infty}^{0}g_1(\lambda,\varepsilon')\exp\left[\frac{i\lambda\varepsilon'}{T}+\frac{\varepsilon'}{2T}\right]f(\varepsilon')d\varepsilon'\ , \tag{82}$$

which is equivalent to the equation

$$f_+(\lambda)+G(\lambda)f_-(\lambda)=-\frac{\gamma}{\omega}\ln\frac{U_0}{T}g_0(\lambda)\times\left[(\lambda^2+\tfrac{1}{4})\left[i\Delta\lambda-i\frac{\partial}{\partial\lambda}\right]-i\lambda-\frac{1}{2}\right]f_-(\lambda)\ . \tag{83}$$

In the correction term, one has to substitute $f_-(\lambda)$ by Eq. (68). Then, with use of the decomposition of $G(\lambda)$, one separates the equation into analytical terms in the upper and lower half-planes of λ and makes use of the relationship

$$A(\Delta)=f_+(i/2)\ . \tag{84}$$

For the function $A_1(\Delta)$, defined by Eq. (15), one obtains

$$A_1(\Delta)=A_0(\Delta)\Delta\left\{\frac{g_0(\lambda)}{G_+(\lambda)}\left[(\lambda^2+\tfrac{1}{4})\left[i\Delta\lambda-i\frac{\partial}{\partial\lambda}\right]-i\lambda-\frac{1}{2}\right]\frac{i}{G_-(\lambda)(\lambda+i/2)}\right\}_+(i/2)\ , \tag{85}$$

where the notation $\{\ \}_+(i/2)$ means that the expression in the curly brackets must be integrated similarly to the Cauchy expression (63) at $\lambda=i/2$,

$$\{\ \}+(i/2)\equiv\int\frac{d\lambda}{2\pi i}\frac{\{\ \}}{\lambda-i/2}\ . \tag{86}$$

The term with Δ in this expression is odd in λ and therefore gives a vanishing contribution, the product $G_+(\lambda)G_-(\lambda)$ must be substituted by $1-g_0(\lambda)$, and the derivative of $\ln G_-(\lambda)$ can be written in the form

$$\frac{\partial\ln G_-(\lambda)}{\partial\lambda}=-\int\frac{d\lambda'}{2\pi i}\frac{\partial\ln G(\lambda')}{\partial\lambda'}\frac{1}{\lambda'-\lambda+i0}=-\int\frac{d\lambda'}{2\pi i}\frac{g_0(\lambda')}{1-g_0(\lambda')}\frac{2\Delta\lambda'}{\lambda'-\lambda+i0}\ . \tag{87}$$

The expression for $A_1(\Delta)$ simplifies then to the following one:

$$A_1(\Delta)=A_0(\Delta)\Delta\int\frac{d\lambda}{2\pi}\frac{g_0(\lambda)}{1-g_0(\lambda)}\times\int\frac{d\lambda'}{2\pi}\frac{g_0(\lambda')}{1-g_0(\lambda')}\frac{2\Delta\lambda'}{\lambda'-\lambda+i0}\ . \tag{88}$$

Symmetrization in λ,λ' is equivalent to the substitution of the latter factor by Δ, which gives the final result

$$A_1(\Delta)=A_0(\Delta)\Phi^2(\Delta)\ , \tag{89}$$

where the function $A_0(\Delta)$ is defined by Eq. (12),

$$\Phi(\Delta)=\Delta\int\frac{d\lambda}{2\pi}\frac{g_0(\lambda)}{1-g_0(\lambda)}=\int\frac{d\lambda}{2\pi}\frac{\Delta}{\exp[\Delta(\lambda^2+\frac{1}{4})]-1}\ . \tag{90}$$

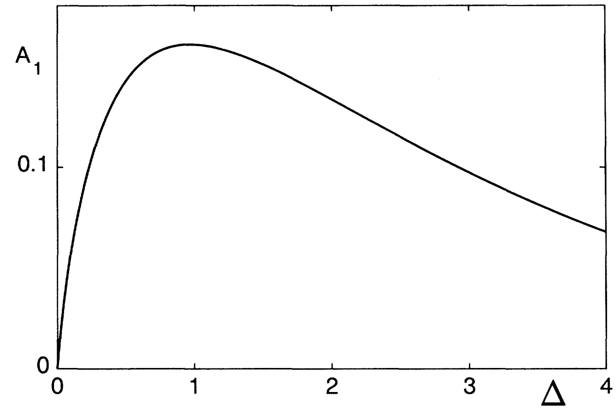

FIG. 1. Coefficient $A_1(\Delta)$ by the leading-logarithmic term.

Asymptotically, this yields

$$\Phi(\Delta)\approx 1+\left[\frac{\Delta}{\pi}\right]^{1/2}\sum_{n=1}^{\infty} n\left[\frac{1}{n^{1/2}}-\frac{1}{2n^{3/2}}-\frac{1}{(n+1)^{1/2}}\right]$$
$$\approx 1-0.407\Delta^{1/2};\quad \Delta \ll 1\ , \tag{91}$$

$$\Phi(\Delta)\approx\frac{1}{2}\left[\frac{\Delta}{\pi}\right]^{1/2}\exp\left[-\frac{\Delta}{4}\right];\quad \Delta\gg 1\ . \tag{92}$$

With an account of the asymptotical behavior of the function $A_0(\Delta)$ one obtains

$$A_1(\Delta)\approx\Delta-1.63\Delta^{3/2};\quad \Delta\ll 1\ , \tag{93}$$

$$A_1(\Delta)\approx(\Delta/4\pi)\exp(-\Delta/2);\quad \Delta\gg 1\ . \tag{94}$$

The function $A_1(\Delta)$ is depicted in Fig. 1.

VII. REFLECTED-PARTICLE CONTRIBUTION

As shown in Sec. III, in a narrow region of the phase space,

$$|p-m\omega x|\sim(\gamma m T/\omega)^{1/2}\ , \tag{95}$$

the distribution function acquires a fine structure due to the effects of friction and thermal noise. Outside of this region, the solution of the Fokker-Planck equation is correctly approximated by the solution of the integral equation derived in Sec. IV. Matching these two solutions in the region $T\gg\varepsilon\gg\gamma T/\omega$, where both of them are applicable, yields the following expression for the distribution function:

$$f(p,x)=f_B\left[\frac{1}{2\pi m\gamma T}\right]^{1/2}\int_{-\infty}^{p-m\omega x}\exp\left[-\frac{\omega u^2}{2m\gamma T}\right]du\ , \tag{96}$$

where f_B is a limiting value of the function $f(\varepsilon)$ at small energies,

$$f_B\equiv f(\varepsilon\to 0)\ . \tag{97}$$

The function (96) provides correct boundary conditions for the distribution functions of the right- and left-going particles at the turning points ($p=0$) for $\varepsilon<0$. On the other hand, for $\varepsilon>0$ (actually, for $\varepsilon>\gamma T/\omega$) and $p<0$ this function is vanishing, which means that no particles enter the potential well from the outside.

Due to the weakness of noise, the recrossing particles occupy a narrow region of the phase space. To take them into account, one has to make use of the small parameter $\gamma/\omega\ll 1$. In a zeroth-order approximation in this parameter, the function $f(p,0)$ is given by $f_B\Theta(p)$. A correction to the decay rate is given then by the integral [see also Eq. (44)]

$$\left[\frac{1}{\tau}\right]^{(1)}=\int_{-\infty}^{\infty}[f(p,0)-f_B\Theta(p)]\frac{p}{m}dp\ . \tag{98}$$

The distinction between the right- and left-going particles becomes clear cut at $x<0$, $|x|\gg(\gamma T/m\omega^2)^{1/2}$, when the distribution of the reflected particles can be approximated by the function

$$f^{\rm refl}(\varepsilon)=f\varepsilon\Theta(-\varepsilon)+\frac{\gamma}{2\omega}f_B T\delta_D(\varepsilon);\quad |\varepsilon|\ll T,\delta\ . \tag{99}$$

Similar to Sec. IV, the function $f(\varepsilon)$ is obtained via one-sided convolution of this function with the kernel $g_0(\varepsilon-\varepsilon)$, which gives a closed integral equation for $f(\varepsilon)$. Expanding the distribution function in the parameter γ/ω, one obtains for the first-order correction $f^{(1)}(\varepsilon)$ the nonuniform integral equation

$$f^{(1)}(\varepsilon)=\int_{-\infty}^{0}g_0(\varepsilon-\varepsilon')f^{(1)}(\varepsilon')d\varepsilon'+\frac{\gamma}{2\omega}f_B T g_0(\varepsilon)\ . \tag{100}$$

The correction to the decay rate is then given by the expression

$$\left[\frac{1}{\tau}\right]^{(1)}=-\frac{\gamma}{2\omega}f_B T+\int_0^{\infty}f^{(1)}(\varepsilon)d\varepsilon\ , \tag{101}$$

where the first term is due to the noise-induced recrossings, whereas the second term is due to the outgoing flux of the initially reflected particles.

Before solving Eq. (100), it is useful to find an explicit expression for the quantity f_B defined by Eq. (97). The inverse Fourier transformation yields

$$f(\varepsilon)=\frac{\Omega}{2\pi T}\exp\left[\frac{U_0}{T}\right]\int[f_+(\lambda)+f_-(\lambda)]\times\exp\left[-\frac{i\lambda\varepsilon}{T}-\frac{\varepsilon}{2T}\right]\frac{d\lambda}{2\pi}\ . \tag{102}$$

This expression should be considered a symbolic one, since the functions $f_+(\lambda)$ and $f_-(\lambda)$ are actually the results of two different Laplace transformations. Therefore, integration in λ for these two functions must be carried out along different contours, going correspondingly above and below their singular points. The function $f_+(\lambda)$ is analytical in the upper half-plane of complex λ. Hence, the real axis of λ can be used as the contour of integration of Eq. (102). In contrast, the function $f_-(\lambda)$ has a pole at $\lambda=-i/2$, and the contour of integration must be placed below this point. In order to shift this contour to the real axis of λ, one has to take into account the residue at the singular point $\lambda=-i/2$. Finally, one obtains

$$f(\varepsilon)=\frac{\Omega}{2\pi T}\exp\left[-\frac{\varepsilon+U_0}{T}\right]\times\left\{1+\int_{-\infty}^{\infty}[f_+(\lambda)+f_-(\lambda)]\times\exp\left[-\frac{i\lambda\varepsilon}{T}+\frac{\varepsilon}{2T}\right]\frac{d\lambda}{2\pi}\right\} . \quad (103)$$

Using Eqs. (67) and (68) for $f_+(\lambda)$ and $f_-(\lambda)$, their sum can be expressed through $G_-(\lambda)$. To calculate f_B, it is sufficient to substitute in Eq. (103) $\varepsilon=0$, which yields

$$f_B=\frac{\Omega}{2\pi T}[1-I(\Delta)]\exp\left[-\frac{U_0}{T}\right] , \quad (104)$$

where

$$I(\Delta)\equiv A_0^{1/2}(\Delta)\int\frac{d\lambda}{2\pi}\frac{ig_0(\lambda)}{(\lambda+i/2)G_-(\lambda)} . \quad (105)$$

In an extremely underdamped regime, this expression yields

$$I(\Delta)\approx 1-1.0\Delta^{1/2},\quad \Delta\ll 1 . \quad (106)$$

For large Δ one obtains

$$I(\Delta)\approx(\pi\Delta)^{1/2}\exp(-\Delta/4) . \quad (107)$$

In order to solve Eq. (100), we resort again to the one-sided Fourier transformations (56), obtaining the equation

$$f_+^{(1)}(\lambda)+G(\lambda)f_-^{(1)}(\lambda)=\frac{\gamma}{2\omega}[1-I(\Delta)]g_0(\lambda) . \quad (108)$$

It is easily solved by the Wiener-Hopf method with the result

$$f_+^{(1)}(\lambda)=\frac{\gamma}{2\omega}[1-I(\Delta)]G_+(\lambda)\int\frac{d\lambda'}{2\pi i}\frac{g_0(\lambda')/G_+(\lambda')}{\lambda'-\lambda-i0} . \quad (109)$$

The integral in Eq. (101) is proportional to $f_+^{(1)}(i/2)$. Making use of the relations $G_+(\lambda)G_-(\lambda)=1-g_0(\lambda)$, $G_+(i/2)=A_0^{1/2}(\Delta)$ and the representation (105), one can express the result in terms of the function $I(\Delta)$,

$$f_+^{(1)}(i/2)=\frac{\gamma}{2\omega}I(\Delta)[1-I(\Delta)] . \quad (110)$$

The final result for the variation of the preexponential factor $A(\gamma/\omega,T/U_0)$ looks like

$$A^{(1)}=-\frac{\gamma}{2\omega}[1-I(\Delta)]^2\equiv-\frac{T}{U_0}\frac{U_0}{\omega S}\frac{\Delta}{2}[1-I(\Delta)]^2 . \quad (111)$$

Comparison with Eq. (15) shows that this correction contributes into the function $B_1(\Delta)$. We denote this contribution through $B_1^{(r)}(\Delta)$ as a reminder that it comes from the reflection-recrossing processes

$$B_1^{(r)}(\Delta)=\frac{\Delta}{2}[1-I(\Delta)]^2 . \quad (112)$$

VIII. CORRECTIONS TO THE GREEN FUNCTION BEYOND THE LOGARITHMIC APPROXIMATION

In Sec. V, the leading-logarithmic correction $g_1^{\rm LL}(\varepsilon,\varepsilon')$ to the kernel of the integral equation was derived, which was sufficient for the calculation of the function $A_1(\Delta)$. To calculate the function $B_1(\Delta)$, one needs to derive the kernel $g_1(\varepsilon,\varepsilon')$ more accurately. Introducing a coordinate $\tilde{x}$ by the inequalities

$$(T/m\omega^2)^{1/2}\ll|\tilde{x}|\ll|x_1| , \quad (113)$$

one can split this problem into the following two. In the major part of the potential well, $x_1<x<\tilde{x}$, the function $g_1(\varepsilon,\varepsilon')$ can be calculated with the use of an expansion in the small ratio $|\varepsilon/U(x)|$. The result will be denoted by $g_1^{\rm BL}(\varepsilon,\varepsilon',\tilde{x})$, keeping in mind that this is a beyond-logarithmic correction to the function $g_1^{\rm LL}(\varepsilon,\varepsilon')$. In the vicinity of the potential barrier (VB), i.e., between $\tilde{x}$ and the turning points $x(\varepsilon)$, $x(\varepsilon')$, one can use a parabolic approximation for $U(x)$ and, in view of a relative narrowness of these regions, solve the Fokker-Planck equation iteratively. As a reminder of its origin, this contribution will be denoted by $g_1^{\rm VB}(\varepsilon,\varepsilon',\tilde{x})$. The final result for the part of $g_1(\varepsilon,\varepsilon')$ contributing to the function $B_1(\Delta)$ looks like

$$g_1^{B}(\varepsilon,\varepsilon')=g_1^{\rm BL}(\varepsilon,\varepsilon',\tilde{x}) . \quad (114)$$

Dependence on $\tilde{x}$ will cancel out, which justifies the introduction of $\tilde{x}$ as an auxiliary parameter. The functions $g_1^{\rm BL}$ and $g_1^{\rm VB}$ will be calculated separately in two next subsections.

A. Major part of the potential well

To derive an expression for $g_1^{\rm BL}(\varepsilon,\varepsilon',\tilde{x})$, one has to calculate more accurately the integrals on the right-hand side of Eq. (78). There are two different integrals. The first one, after subtraction of the term already accounted for in the function $g_1^{\rm LL}(\varepsilon,\varepsilon')$, can be written as

$$2\gamma\int_{x_1}^{\tilde{x}}\left[-\frac{m}{2U(x)}\right]^{1/2}dx-\frac{\gamma}{\omega}\ln\frac{U_0}{T}=\frac{\gamma}{\omega}\left[C_U+\ln\frac{T}{m\omega^2\tilde{x}^2}\right] , \quad (115)$$

where the dimensionless number C_U is given by Eq. (29). The second integral can be expressed through the same number C_U,

$$\gamma\oint_{\bar{x}}^{\bar{x}}\left[-\frac{m}{2U(x)}\right]^{1/2}\frac{\delta(x)}{T}dx-\frac{\gamma}{\omega}\Delta\ln\frac{U_0}{T}\equiv\gamma^2\int_{x_1}^{\bar{x}}\left[-\frac{m}{2U(x)}\right]^{1/2}\left[\int_x^{\bar{x}}+\int_{x_1}^{\bar{x}}\right][-2mU(x')]^{1/2}dx'-\frac{\gamma}{\omega}\Delta\ln\frac{U_0}{T}$$
$$=2\gamma^2\int_{x_1}^{\bar{x}}\left[-\frac{m}{2U(x)}\right]^{1/2}\int_{x_1}^{\bar{x}}[-2mU(x')]^{1/2}dx'-\frac{\gamma}{\omega}\Delta\ln\frac{U_0}{T}$$
$$\approx\frac{\gamma}{2\omega}\Delta\left[C_U+\ln\frac{T}{m\omega^2\bar{x}^2}\right], \tag{116}$$

where we have neglected a small term on the relative order $(\bar{x}/x_1)^2\ll 1$. The final result for the contribution from the major part of the potential well can now be written as follows:

$$g_1^{\rm BL}(\varepsilon,\varepsilon',\bar{x})=-\frac{\gamma}{\omega}\left[C_U+\ln\frac{T}{m\omega^2\bar{x}^2}\right]\left\{\frac{\varepsilon+\varepsilon'}{T}\left[\frac{1}{8}+\frac{1}{4\Delta}-\frac{(\varepsilon-\varepsilon')^2}{8\Delta^2T^2}\right]-\frac{1}{2}\right\}. \tag{117}$$

B. Vicinity of the barrier top

To find the contribution into $g_1(\varepsilon,\varepsilon')$ from the region $[\bar{x},x(\varepsilon)]$, one can use the equation

$$\frac{\partial g(\varepsilon,\varepsilon';x,\bar{x})}{\partial x}=\gamma\frac{\partial}{\partial\varepsilon}(2m\varepsilon+m^2\omega^2x^2)^{1/2}\left[T\frac{\partial}{\partial\varepsilon}+1\right]g_0(\varepsilon-\varepsilon'), \tag{118}$$

where the function $g_0(\varepsilon-\varepsilon')$ is substituted into the right-hand side as a zeroth-order approximation. Integrations in x must be carried out from $\bar{x}$ to $x(\varepsilon)$, where

$$x(\varepsilon)=0;\quad \varepsilon>0, \tag{119}$$

$$x(\varepsilon)=-(-2\varepsilon/m)^{1/2}/\omega;\quad \varepsilon<0. \tag{120}$$

The result is

$$g[\varepsilon,\varepsilon';x(\varepsilon),\bar{x}]=g(\varepsilon,\varepsilon';\bar{x},\bar{x})+\frac{\gamma}{2\omega}\frac{\partial}{\partial\varepsilon}\left[m\omega^2\bar{x}^2+\varepsilon+\varepsilon\ln\frac{2m\omega^2\bar{x}^2}{|\varepsilon|}\right]\left[T\frac{\partial}{\partial\varepsilon}+1\right]g_0(\varepsilon-\varepsilon').$$

The term $\propto\bar{x}^2$ should be omitted, since it was already accounted for when deriving $g_0(\varepsilon-\varepsilon')$. Substituting Eq. (52) for this function, performing the differentiation, and separating the common factor $g_0(\varepsilon-\varepsilon')$, one obtains a contribution to $g_1^{\rm VB}(\varepsilon,\varepsilon';\bar{x})$. A similar contribution comes in from the starting piece of the trajectory $\bar{x}<x<x(\varepsilon')$, where one must use the equation

$$\frac{\partial g(\varepsilon,\varepsilon';\bar{x},x')}{\partial x'}=\gamma\left[T\frac{\partial}{\partial\varepsilon'}-1\right](2m\varepsilon'+m^2\omega^2x'^2)\frac{\partial}{\partial\varepsilon'}g_0(\varepsilon-\varepsilon'). \tag{121}$$

Combining these two contributions one obtains

$$g_1^{\rm VB}(\varepsilon,\varepsilon';\bar{x})=-\frac{\gamma}{\omega}\left\{\left[\frac{\varepsilon+\varepsilon'}{T}\left[\ln\frac{2m\omega^2\bar{x}^2}{T}+1\right]-\frac{\varepsilon}{T}\ln\frac{|\varepsilon|}{T}-\frac{\varepsilon'}{T}\ln\frac{|\varepsilon'|}{T}\right]\left[\frac{1}{8}+\frac{1}{4\Delta}-\frac{(\varepsilon-\varepsilon')^2}{8\Delta^2T^2}\right]\right.$$
$$\left.+\frac{1}{4}\left[\mathrm{sgn}\varepsilon+\mathrm{sgn}\varepsilon'-2-2\ln 2-2\ln\frac{m\omega^2\bar{x}^2}{T}+\ln\frac{|\varepsilon|}{T}+\ln\frac{|\varepsilon'|}{T}-\frac{\varepsilon-\varepsilon'}{T}\left[\ln\left|\frac{\varepsilon}{\varepsilon'}\right|+\mathrm{si}n\varepsilon-\mathrm{si}n\varepsilon'\right]\right]\right\}. \tag{122}$$

According to the definition (114), this expression should be added to Eq. (117). Dependence on the auxiliary parameter $\bar{x}$ will then cancel out and the final result can be represented in the following form:

$$g_1^B(\varepsilon,\varepsilon')=-\frac{T}{U_0}\frac{U_0}{\omega S}(C_U+1+\ln 2)\left\{\frac{\varepsilon+\varepsilon'}{T}\left[\frac{1}{8}+\frac{1}{4\Delta}-\frac{(\varepsilon-\varepsilon')^2}{8\Delta^2T^2}\right]-\frac{1}{2}\right\}-\frac{T}{U_0}\frac{U_0}{\omega S}\mathcal{K}(\varepsilon,\varepsilon'), \tag{123}$$

where

$$\mathcal{K}(\varepsilon,\varepsilon')\equiv\Delta\left[\frac{\varepsilon}{T}\ln\frac{|\varepsilon|}{T}+\frac{\varepsilon'}{T}\ln\frac{|\varepsilon'|}{T}\right]\left[\frac{1}{8}+\frac{1}{4\Delta}-\frac{(\varepsilon-\varepsilon')^2}{8\Delta^2T^2}\right]$$
$$-\frac{1}{4}\left[\ln\frac{|\varepsilon|}{T}+\ln\frac{|\varepsilon'|}{T}+\text{sgn}\varepsilon+\text{sgn}\varepsilon'-\frac{\varepsilon-\varepsilon'}{T}\left[\ln\left|\frac{\varepsilon}{\varepsilon'}\right|+\text{sgn}\varepsilon'-\text{sgn}\varepsilon'\right]\right]. \quad (124)$$

From this expression one concludes that the function $f(\varepsilon)$ behaves at small ε in a singular way, particularly, it has a finite jump at $\varepsilon=0$ due to the term $\propto\text{sgn}\varepsilon$ and a logarithmic divergence. These singularities reflect a qualitative difference between the escaping ($\varepsilon>0$) and reflected ($\varepsilon<0$) particles. For energies $\sim\gamma T/\omega$, these singularities will be smeared out similarly to Eq. (96).

The correction to the function $B_1(\Delta)$ due to the first term in Eq. (123) is expressed through the function $A_1(\Delta)$, since this term differs from Eq. (81) only by a constant factor. Therefore, $B_1(\Delta)$ can be represented in the form

$$B_1(\Delta)=(\Delta/2)[1-I(\Delta)]^2+A_1(\Delta)(C_U+1+\ln 2)+\int_0^\infty f^{(1)}(\varepsilon)d\varepsilon\ , \quad (125)$$

where the function $f^{(1)}(\varepsilon)$ gives a correction to the distribution function $f(\varepsilon)$ due to the last term of Eq. (123).

IX. PERTURBED INTEGRAL EQUATION AND ITS SOLUTION

The function $f^{(1)}(\varepsilon)$ is governed by the integral equation

$$f^{(1)}(\varepsilon)-\int_{-\infty}^0 g_0(\varepsilon-\varepsilon')f^{(1)}(\varepsilon')d\varepsilon'=\int\frac{d\lambda'}{2\pi}f_-(\lambda')\int_{-\infty}^\infty g_0(\varepsilon-\varepsilon')\mathcal{K}(\varepsilon,\varepsilon')\exp\left[-\frac{i\lambda'\varepsilon'}{T}-\frac{\varepsilon'}{2T}\right]d\varepsilon'\ . \quad (126)$$

The integral in ε' on the right-hand side of this equation has been extended to infinity, since contribution from the positive ε' vanishes identically due to analytical properties of the function $f_-(\lambda')$ [see Eq. (68)]. Introducing the Fourier transformations in the standard way by Eq. (56), one obtains

$$\int_0^\infty f^{(1)}(\varepsilon)d\varepsilon=f_+^{(1)}(i/2)\ . \quad (127)$$

To represent the final result in a compact form, we introduce the Green function of the integral equation,

$$\mathcal{G}(\varepsilon,\varepsilon')=\int_{-\infty}^0 g_0(\varepsilon,\varepsilon'')\mathcal{G}(\varepsilon'',\varepsilon')=\delta_D(\varepsilon-\varepsilon')\exp\left[-\frac{\varepsilon}{2T}\right]. \quad (128)$$

In the Fourier representation,

$$\mathcal{G}_+(\lambda,\varepsilon')-[1-g_0(\lambda)]\mathcal{G}_-(\lambda,\varepsilon')=\exp\left[\frac{i\lambda\varepsilon'}{T}\right]. \quad (129)$$

The expression for $\mathcal{G}_+(i/2,\varepsilon')$, needed for the calculation of $f_+^{(1)}(i/2)$, is given by the function

$$\mathcal{G}(\varepsilon')=A^{1/2}(\Delta)\int\frac{d\lambda}{2\pi i}\frac{\exp(i\lambda\varepsilon'/T)}{(\lambda-i/2)G_+(\lambda)}\ . \quad (130)$$

With the use of these results, one obtains

$$f_+^{(1)}(i/2)=A_0(\Delta)\int\frac{d\lambda}{2\pi}\int\frac{d\lambda'}{2\pi}\frac{\tilde{\mathcal{K}}(\lambda,\lambda')}{(\lambda-i/2)G_+(\lambda)(\lambda'+i/2)G_-(\lambda')}\ , \quad (131)$$

where

$$\tilde{\mathcal{K}}(\lambda,\lambda')\equiv-\int\int d\varepsilon\,d\varepsilon' g_0(\varepsilon-\varepsilon')\mathcal{K}(\varepsilon,\varepsilon')\exp\left[\frac{i\lambda\varepsilon-i\lambda'\varepsilon'}{T}+\frac{\varepsilon-\varepsilon'}{2T}\right]. \quad (132)$$

To proceed further, we introduce the convenient representation

$$g_0(\varepsilon-\varepsilon')\mathcal{K}(\varepsilon,\varepsilon')=\frac{\Delta}{2}\left[\frac{\partial}{\partial\varepsilon}\varepsilon\ln\frac{|\varepsilon|}{T}\left[T\frac{\partial}{\partial\varepsilon}+1\right]+\left[T\frac{\partial}{\partial\varepsilon'}-1\right]\varepsilon'\ln\frac{|\varepsilon'|}{T}\frac{\partial}{\partial\varepsilon'}\right]g_0(\varepsilon-\varepsilon')\ . \quad (133)$$

Substituting this expression into Eq. (132) gives the result

$$\tilde{\mathcal{K}}(\lambda,\lambda')=-(\Delta/2)J(\lambda-\lambda')(\lambda-i/2)(\lambda'+i/2)[g_0(\lambda)+g_0(\lambda')]\ , \quad (134)$$

where a singular function $J(\lambda)$ is defined by the integral

$$J(\lambda)\equiv\int_{-\infty}^{\infty} x\ln|x|\exp(i\lambda x)dx\ . \qquad (135)$$

This function has a singular point at $\lambda=0$, and we have to consider the result of integration of this function with a function $\varphi(\lambda)$ analytical near the real axis of λ.

In order to elucidate the derivation, we investigate a simpler integral,

$$\int_{-\infty}^{\infty}\varphi(\lambda)\frac{d\lambda}{2\pi}\int_{-\infty}^{\infty}\ln|x|\exp(i\lambda x)dx=\int_{C_1}\varphi(\lambda)\frac{d\lambda}{2\pi}\int_0^{\infty}\ln|x|\exp(i\lambda x)dx+\int_{C_2}\varphi(\lambda)\frac{d\lambda}{2\pi}\int_{-\infty}^{0}\ln|x|\exp(i\lambda x)dx\ , \qquad (136)$$

where the contour of integration C_1 (C_2) is placed above (below) the real axis of λ. Performing integrals in x, one obtains the integrals

$$\int_{C_1}\varphi(\lambda)\frac{C+\ln(-i\lambda)}{i\lambda}\frac{d\lambda}{2\pi}+\int_{C_2}\varphi(\lambda)\frac{C+\ln(i\lambda)}{-i\lambda}\frac{d\lambda}{2\pi}=-(C+\ln\rho)\varphi(0)-\left[\int_{-\infty}^{-\rho}+\int_{\rho}^{\infty}\right]\frac{\varphi(\lambda)}{|\lambda|}\frac{d\lambda}{2}\ , \qquad (137)$$

where

$$C\equiv-\int_0^{\infty}e^{-x}\ln x\,dx\approx 0.5772\ . \qquad (138)$$

Calculating the integrals on the right-hand side of Eq. (137) by parts, one obtains

$$\int_{-\infty}^{\infty}\varphi(\lambda)\frac{d\lambda}{2\pi}\int_{-\infty}^{\infty}\ln|x|\exp(i\lambda x)dx=-C\varphi(0)+\tfrac{1}{2}\int_{-\infty}^{\infty}\frac{d\varphi(\lambda)}{d\lambda}\ln|\lambda|\mathrm{sgn}\lambda\,d\lambda\ . \qquad (139)$$

For the function $J(\lambda)$, a similar calculation yields

$$\int_{-\infty}^{\infty}\varphi(\lambda)J(\lambda)\frac{d\lambda}{2\pi}=-iC\varphi'(0)+i\pi\int_{-\infty}^{\infty}\frac{d^2\varphi(\lambda)}{d\lambda^2}\ln|\lambda|\mathrm{sgn}(\lambda)\frac{d\lambda}{2\pi}\ . \qquad (140)$$

Substitution of Eqs. (134) and (140) into Eq. (131) yields

$$f_+^{(1)}(i/2)=-CA_1(\Delta)+D(\Delta)\ , \qquad (141)$$

where

$$D(\Delta)\equiv A_0(\Delta)\Delta\frac{i\pi}{2}\int\int\ln|\lambda-\lambda'|\mathrm{sgn}(\lambda-\lambda')\frac{d^2}{d\lambda\,d\lambda'}\frac{g_0(\lambda)+g_0(\lambda')}{G_+(\lambda)G_-(\lambda')}\frac{d\lambda}{2\pi}\frac{d\lambda'}{2\pi}\ . \qquad (142)$$

In an extremely underdamped limit, $\Delta\ll1$, one can substitute $A_0(\Delta)\approx\Delta$, $A_1(\Delta)\approx\Delta$, $g_0(\lambda)\approx1$, and make use of Eq. (64) for $G_\pm(\lambda)$. Then for the function $D(\Delta)$ one obtains

$$D(\Delta)\approx i\pi\Delta\int\int\frac{d\lambda}{2\pi}\frac{d\lambda'}{2\pi}\frac{\ln|\lambda-\lambda'\mathrm{sgn}(\lambda-\lambda')}{(\lambda+i/2)^2(\lambda'-i/2)^2}=\Delta\ . \qquad (143)$$

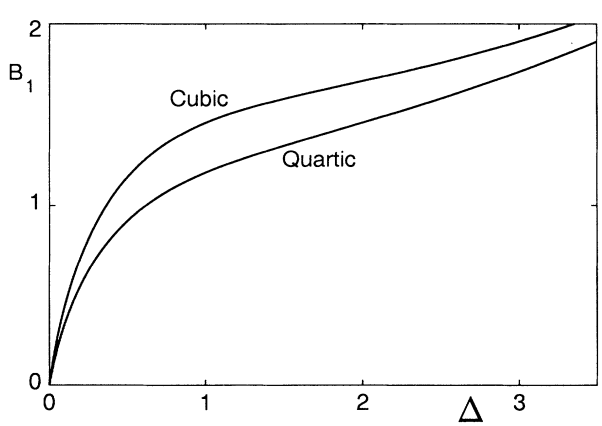

FIG. 2. Coefficient in the beyond-logarithmic approximation $B_1(\Delta)$ for cubic and quartic potentials.

This yields the asymptotics

$$\int_0^{\infty}f^{(1)}(\varepsilon)d\varepsilon\approx-C\Delta+\Delta,\quad \Delta\ll1 \qquad (144)$$

which after substitution into Eq. (125) reproduces Eq. (34). The final result for $B_1(\Delta)$ looks like

$$B_1(\Delta)=(\Delta/2)[1-I(\Delta)]^2+(C_U+1+\ln2-C)A_1(\Delta)+D(\Delta)\ . \qquad (145)$$

The function $B_1(\Delta)$ for the cubic, Eq. (35), and the quartic, Eq. (38), potentials is shown in Fig. 2.

X. QUANTITATIVE RESULTS FOR THE TURNOVER PROBLEM

The results given by Eqs. (12), (89), and (145) are sufficient for calculation of the corrected preexponential factor from Eq. (15). It should be emphasized that the results obtained are exact in what concerns the calculation of A up to terms of the order of T/U_0. Similar to [5], we find it convenient to write down an interpolating expression which is correct so long as terms of the order $(\gamma/\omega)^2$ can be neglected and reproduce the Kramers result for $\gamma/\omega\sim1$,

$$A(\gamma/\omega, T/U_0) = A_0(\Delta)\left[1+\frac{\gamma^2}{4\omega^2}\right]^{1/2} - \frac{T}{U_0}\frac{U_0}{\omega S}\left[A_1(\Delta)\ln\frac{U_0}{T} + B_1(\Delta)\right] . \quad (146)$$

It is worth it to point out that in the range $\Delta \gg 1$ the term with $B_1(\Delta)$ correctly reproduces the decrease of A linear in $\gamma/2\omega$, as it follows from Eqs. (45) and (48). When combined with the first term in Eq. (146), where $A_0 \approx 1$, this yields the Kramers result

$$A(\gamma/\omega) = (1+\gamma^2/4\omega^2)^{1/2} - \gamma/2\omega . \quad (147)$$

Therefore, Eq. (146) describes the turnover behavior of the prefactor A with account of corrections of the order of T/U_0 in a weak-to-intermediate regime of friction. It will be shown in the next section that corrections in the same small parameter in the regime of an intermediate-to-strong friction are always negligible. Therefore, Eq. (146) has to be considered as fairly satisfactory for arbitrary friction. Numerical results for the cubic potential (35) are shown in Fig. 3 for several values of the parameter T/U_0 simultaneously with the curves for the simplest interpolation expression [5],

$$A(\gamma/\omega, T/U_0) = A_0(\Delta)\left[\left[1+\frac{\gamma^2}{4\omega^2}\right]^{1/2} - \frac{\gamma}{2\omega}\right] . \quad (148)$$

The final conclusion is that, for the regime of a not-too-weak friction, the simplified Eq. (148) gives surprisingly good results down to rather low barrier heights $U_0 \sim T$. For instance, the magnitude and position of the maximum of A as a function of γ/ω are only weakly influenced by the corrections. For $T/U_0 = 1.0$, the position of the maximum of A shifts from $\gamma/\omega \approx 0.76$ to $\gamma/\omega \approx 0.58$, whereas its magnitude is only decreased by 10%. For $T/U_0 = 0.5$, the relative shift of the maximum

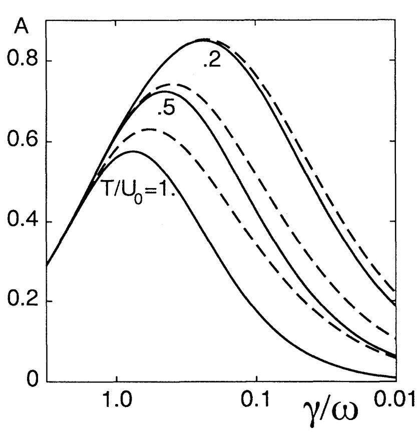

FIG. 3. Turnover behavior of the preexponential factor A for the cubic potential (35). The dashed curves correspond to Eq. (148).

position is about 10%, its magnitude decreases less than by 3%.

In the regime of a weak friction, the small numerical factor in Eq. (3.1),

$$U_0/\omega S = 5/36 \approx \tfrac{1}{7} ,$$

is compensated by the second numerical factor,

$$C_U + 2 + \ln 2 - C \approx 7.49 ,$$

so that for the cubic potential form Eqs. (31), (36), and (37) one obtains

$$A \approx \Delta\left[1 - 1.0\frac{T}{U_0} - \frac{5}{36}\frac{T}{U_0}\ln\frac{U_0}{T}\right], \quad \Delta \ll 1 . \quad (149)$$

According to general properties of asymptotic expansions, one expects that Eq. (149) gives a good approximation for A in the region $T/U_0 < 0.2$. Hence, in the case of high barriers, $U_0 > 5T$, one can use Eq. (148) as a zero approximation and estimate the finite-barrier corrections with the use of Eq. (146). For $U_0 < 5T$, the preexponential factor A becomes dependent both on the height and the shape of the barrier. Fortunately, for low barriers the activated decay rate can be efficiently calculated by computer simulations [9,11,12].

XI. INTERMEDIATE-TO-STRONG FRICTION REGIME

In a strong-friction regime, $\Delta \gg 1$, the parameter γ/ω becomes eventually of the order unity and one has to consider corrections in the remaining small parameter T/U_0. As shown by Kramers, for $\gamma \sim \omega$ the basic result can be obtained in a parabolic approximation for the potential $U(x)$ near the top of the barrier. To calculate corrections to this result, one has to expand the potential up to cubic and/or quartic terms,

$$U(x) \approx -\frac{m\omega^2 x^2}{2} + U^{(3)}\frac{x^3}{6} + U^{(4)}\frac{x^4}{24} . \quad (150)$$

It will be shown below that a linear contribution of $U^{(3)}$ vanishes, whereas the second-order term in this parameter has the same order of magnitude as the linear-in-$U^{(4)}$ contribution. The anticipated expression for the preexponential factor A can then be written in the form

$$A = \left[1+\frac{\gamma^2}{4\omega^2}\right]^{1/2} - \frac{\gamma}{2\omega} - \frac{T}{U_0}\left[C_3 a_3\left[\frac{\gamma}{\omega}\right] + C_4 \alpha_4\left[\frac{\gamma}{\omega}\right]\right] , \quad (151)$$

where the dependence on the shape of the potential enters through the numerical factors

$$C_3 \equiv \frac{[U^{(3)}]^2 U_0}{(m\omega^2)^3} , \quad (152)$$

$$C_4 \equiv \frac{U^{(4)} U_0}{(m\omega^2)^2} , \quad (153)$$

and $a_n(\gamma/\omega)$ are universal functions. For the cubic potential considered above, $C_3=\frac{2}{3}$, $C_4=\frac{3}{2}$, and for a cosine potential $C_4=2$.

To calculate the functions $a_n(\gamma/\omega)$, we substitute into Eq. (2) the function

$$f(p,x)=\frac{\Omega}{2\pi T}\varphi(p,x)\exp\left[-\frac{p^2}{2mT}-\frac{U(x)}{T}\right], \quad (154)$$

and rewrite it in the form

$$\gamma m T\frac{\partial^2\varphi}{\partial p^2}-\frac{p}{m}\frac{\partial\varphi}{\partial x}-(m\omega^2 x+\gamma p)\frac{\partial\varphi}{\partial p}=-\left[\frac{\partial U}{\partial x}+m\omega^2 x\right]\frac{\partial\varphi}{\partial p} . \quad (155)$$

Following Kramers, we introduce, instead of p, a new variable,

$$u=(p-\alpha m\omega x)(\omega/\alpha\gamma m T)^{1/2} , \quad (156)$$

where

$$\alpha=\left[1+\frac{\gamma^2}{4\omega^2}\right]^{1/2}+\frac{\gamma}{2\omega} . \quad (157)$$

In neglection of the right-hand side of Eq. (155), its solution is independent of x and is given by the error integral,

$$\varphi_0(u)=(2\pi)^{-1/2}\int_{-\infty}^{u}\exp\left[-\frac{v^2}{2}\right]dv . \quad (158)$$

To proceed further, the function $\varphi(x,u)$ is written as

$$\varphi(x,u)=\varphi_0(u)+(2\pi)^{-1/2}\psi(x,u)\exp(-u^2/2) . \quad (159)$$

On the right-hand side of Eq. (155) we substitute

$$\frac{\partial U}{\partial x}+m\omega^2 x=U^{(n)}\frac{x^{n-1}}{(n-1)!} , \quad (160)$$

and consider separately the cases of $n=3$ and 4. The flux of particles is calculated at $x=0$. Hence, it is convenient to rescale the coordinate,

$$x\to x(\alpha^3\gamma T/m\omega^3)^{1/2} , \quad (161)$$

and calculate an expression for $\psi(0,u)$, which does not depend on the scale of x. The resulting equation for $\psi(x,u)$ looks rather compact,

$$\frac{\partial^2\psi}{\partial u^2}-u\frac{\partial\psi}{\partial u}-\psi-(u+\alpha^2 x)\frac{\partial\psi}{\partial x}=-\mu_n x^{n-1}\left[1-u\psi+\frac{\partial\psi}{\partial u}\right], \quad (162)$$

where

$$\mu_n\equiv C_n^{n/2-1}\left[\frac{\gamma T}{\omega U_0}\right]^{n/2-1}\frac{\alpha^{3n/2-1}}{(n-1)!},\quad n=3,4 . \quad (163)$$

The case of $n=4$ is the most simple one, since already the linear term gives a nonvanishing contribution. To calculate it, the function $\psi(x,u)$ must be expanded in powers of x,

$$\psi(x,u)\equiv-\mu_4\sum_{l=0}^{3}P_l(u)x^l , \quad (164)$$

where $P_l(u)$ is the polynomial of u. The resulting system of equations looks like

$$P_l''-uP_l'-(1+\alpha^2 l)P_l-u(l+1)P_{l+1}=\delta l,3 , \quad (165)$$

where $\delta_{n,l}$ is the Kronecker symbol. It can be solved by descending iterations, starting with $P_4=0$. The final result for $P_0(u)$ is

$$P_0(u)=\frac{3u[(u^2+3)(\alpha^2+1)+4]}{4(\alpha^2+1)^2(\alpha+3)(3\alpha^2+1)} . \quad (166)$$

The function a_4 is given by the integral

$$a_4=\frac{\alpha^6}{6}\left[\frac{\gamma}{\omega}\right]^2\int_{-\infty}^{\infty}\exp\left[-\frac{\alpha^2u^2}{2}\right]P_0(u)\frac{udu}{(2\pi)^{1/2}}=\frac{1}{8\alpha}\left[\frac{\gamma}{\omega}\right]^2\frac{1}{(\alpha^2+1)^2} . \quad (167)$$

In the limit of a weak friction, $\gamma\ll\omega$, for the potential (38) one obtains

$$A\approx1-\frac{\gamma}{2\omega}+\frac{1}{8}\left[\frac{\gamma}{\omega}\right]^2\left[1-\frac{3}{8}\frac{T}{U_0}\right] . \quad (168)$$

In the opposite limit,

$$A\approx\frac{\omega}{\gamma}\left[1-\frac{3}{16}\frac{T}{U_0}\frac{\omega^2}{\gamma^2}\right],\quad \gamma/\omega\gg1 . \quad (169)$$

From these expressions one concludes that corrections in the parameter T/U_0 enter with numerical factors smaller than unity, which makes them small even for $T/U_0\sim1$. For a cubic potential, the linear-in-μ_3 contribution to $\psi(u)$ is even in u, so that the integral (167) vanishes. To find the second-order correction, we introduce the expansion

$$\psi(x,u)=-\mu_3\sum_{l=0}^{2}P_l(u)x^l-\mu_3^2\sum_{l=0}^{4}Q_l(u)x^l . \quad (170)$$

The system of equations for $P_l(u)$ and $Q_l(u)$ looks like

$$P_l''-uP_l'-(1+\alpha^2 l)P_l-u(l+1)P_{l+1}=\delta_{l,2} , \quad (171)$$

$$Q_l''-uQ_l'-(1+\alpha^2 l)Q_l-u(l+1)Q_{l+1}=uP_{l-2}-P_{l-2}' . \quad (172)$$

The function $a_3(\gamma/\omega)$ is then given by the integral

$$a_3(\gamma/\omega)=\frac{\alpha^8}{4}\left[\frac{\gamma}{\omega}\right]^2\int\exp\left[-\frac{\alpha^2u^2}{2}\right]Q_0(u)\frac{udu}{(2\pi)^{1/2}} . \quad (173)$$

The numerical results for the functions $a_3(\gamma/\omega)$ and $a_4(\gamma/\omega)$ are shown in Fig. 4. Due to the smallness of these functions, the resulting corrections to Eq. (147) do not exceed 1.5% even at $T/U_0=1$. Therefore, in the regime of an intermediate-to-strong friction, $\gamma/\omega>1$, one

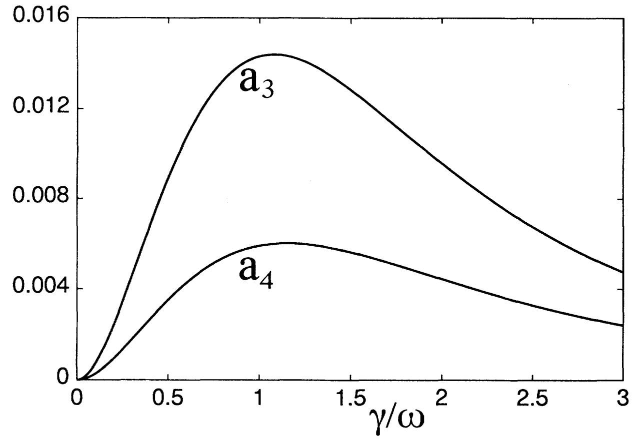

FIG. 4. Dimensionless functions $A_3(\gamma/\omega)$ and $a_4(\gamma/\omega)$.

can always apply Eq. (146).

Experimentally, nearly ideal model systems for the observation of activated decay are provided by Josephson junctions [13,14]. At the present time, superconducting quantum interference devices (SQUID) are becoming more popular in studying the thermally activated decay, since they allow to investigate both one- and two-dimensional processes under controllable conditions [15,16]. Typically, the SQUID's operate in the regime of an intermediate-to-strong friction. Both experimental and numerical stimulation results agree fairly well with the theoretical predictions for one- and two-dimensional activation. No deviations from the Arrhenius law with the simplest expression for the preexponential factor were discovered down to rather low barrier heights, $U_0 \sim 1.5T$ [16].

The results of our calculations provide a quantitative estimation of finite-barrier corrections in the small parameter T/U_0. In the intermediate-to-strong friction regime, these corrections are always negligible, since the functions $a_3(\gamma/\omega)$ and $a_4(\gamma/\omega)$ never exceed 1/70. This conclusion is in agreement with the experimental findings [16]. Near the turnover region, a simple interpolating expression gives satisfactory results both for the position and the height of the maximum of the preexponential factors down to $U_0/T=2$. With account of corrections for a finite-barrier height, this description of the turnover region can be extended down to $U_0/T=1$. In the regime of a weak friction, the finite-barrier corrections become significant for $U_0/T\sim 5$ (see Fig. 3). For lower barriers, the activated decay rate depends nontrivially both on the shape and the height of the potential and can only be calculated numerically [11,12].

Note added in proof. Recently, finite barrier corrections for the activated decay rate have been investigated in the Smoluchowski limit by E. Pollak and P. Talkner, Phys. Rev. E **46**, 922 (1993).

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