Thermal activation in extremely underdamped Josephson-junction circuits

M. Büttiker, E. P. Harris, and R. Landauer
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598
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Noise-activated escape of a particle out of a metastable well was treated by Kramers, who derived results covering the three cases of heavy damping, moderate damping, and extreme underdamping. In the case of extreme underdamping, the escape occurs through diffusive motion along the energy coordinate. We extend Kramers's treatment of this extremely underdamped case to cover a wider range of damping constants, taking into account that at energies just above the barrier peak and within the initial well, the distribution is controlled both by uphill diffusion in energy, and by the flow out of the well. This new result is compared with computer simulations of escape events for the case of Josephson junctions under constant current bias. In addition to a conventional simulation which initially puts the particles at the bottom of the well, a method is developed which requires simulation only in an energy range close to the peak of the barrier.

I. INTRODUCTION

Noise-activated escape from a metastable state was treated in a historic pioneering paper by Kramers.[1] Since that time Kramers's work has been elaborated in many ways, and we can cite only a few items from a long list of such elaborations.[2] Our paper treats the situation depicted in Fig. 1, showing a particle in a sinusoidal potential $V_0(1-\cos\theta)$ supplemented by a driving potential $-F\theta$. The particle obeys an equation of motion,

$$m\ddot{\theta}+\gamma\dot{\theta}=-\frac{dV}{d\theta}+\xi\ , \tag{1.1}$$

where $V=V_0(1-\cos\theta)-F\theta$. In Eq. (1.1), the thermal equilibrium noise ξ obeys $\langle\xi\rangle=0$ and

$$\langle\xi(t)\xi(t')\rangle=2\gamma kT\delta(t-t')\ . \tag{1.2}$$

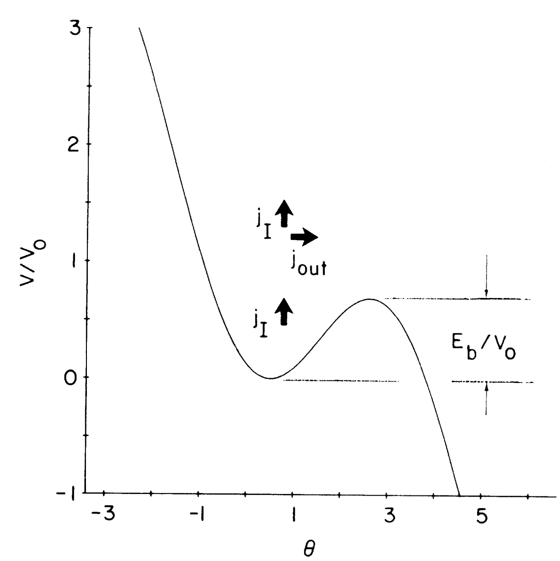

FIG. 1. Potential $V=V_0(1-\cos\theta)-F\theta$ in Eq. (1.1) for $F=\frac{1}{2}V_0$. In the strongly underdamped case, emphasized in this paper, there is a diffusive flux along the action or energy coordinate j_I. For energies above the barrier peak energy E_b, we have, in addition to this vertical current, a horizontal current j_{out} giving the flux out of the well.

Our tilted sinusoidal potential is similar to that of a classical particle in a periodic solid, subject to an external electric field. In that case we can have an equilibrium distribution, if we add walls at each end of the specimen. This results in a polarized nonuniform particle distribution favoring the low-energy end of the specimen, and results in an absence of steady-state transport. Alternatively, we can study a periodic distribution function which does represent transport, as is typically done in conductivity calculations. It is this latter periodic distribution function which is the subject of our discussion. The resulting equations also characterize a Josephson-junction circuit under constant current bias.[3] A particle trapped in a local minimum of the tilted sinusoid will, eventually, under the influence of fluctuations, escape to the right. If the damping is appreciable the escape will be to the next potential minimum. If the damping is low, however, then the particle which gains enough energy to pass one barrier will not lose $2\pi F$ in energy, via damping, while passing over to the next barrier, and thus will continue to move to the right, with high probability. Let us briefly discuss the equation of motion, Eq. (1.1), in the absence of noise. For $G\leq 1.19$, where $G=\gamma/(mV_0)^{1/2}$ is a dimensionless damping constant, there will be a range of F (or a range of currents for the Josephson junction) in which we have bistability.[3] In this range the particle can satisfy the noiseless equations of motion either by sitting quietly at the bottom of a well, or else it can be in a steady state in which θ advances as a periodic function of time (see Fig. 2). The range of bistability is shown in Fig. 3, adapted from Fig. 7 of Ref. 4. These two regimes of local stability will be separated by a separatrix.[5]

In the region of bistability just discussed, fluctuations will induce transitions from the locked state (particle at the bottom of a well; superconducting state) to the running state ($\dot{\theta}>0$; voltage state) and visa versa. The probability for fluctuation-activated escape from the running state, back into the locked state, was evaluated recently[6] and will not be our concern in this paper. In the bistable regime the relative occupation probability of the two kinds of competing states of local stability will be determined, in the stochastic steady state, by a balance in the escape rates. That question has been considered in detail, in a sequence of papers by Risken and Vollmer, of which we cite only a

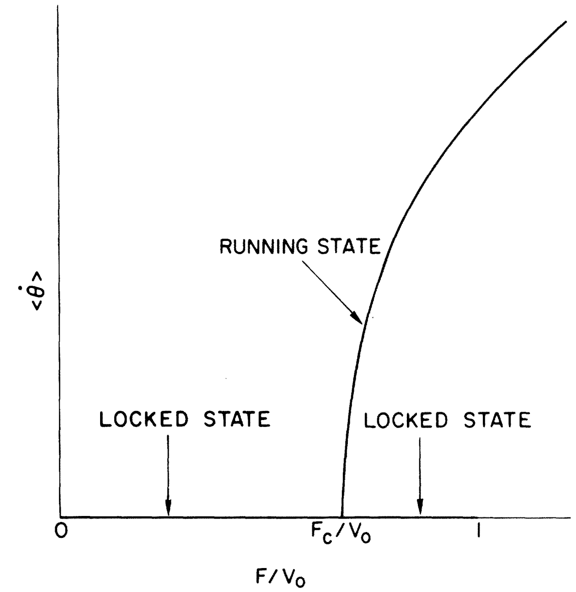

FIG. 2. Stable states of a particle moving in the potential of Fig. 1. The field range $F_c < F < V_0$ allows both a locked state with zero average velocity and a running state with nonzero average velocity.

recent one.[7] Numerical simulations describing the repeated transitions back and forth between local stability and the moving steady state have also been given.[8,9] As in any such situation,[10] as the parameters are changed and a stable state approaches marginality, i.e., the limit of its range of local stability, it is certain to become the less likely state, because it will require very little noise for escape from such a marginal state.

Our concern is with the simplest of these questions, the escape rate from a potential minimum. We will also focus on the *underdamped* case illustrated schematically in Fig. 1. Particles reaching the energy E_b can escape to the right; they are prevented by the potential from going to the left. Thus the net upward flux in energy is also the

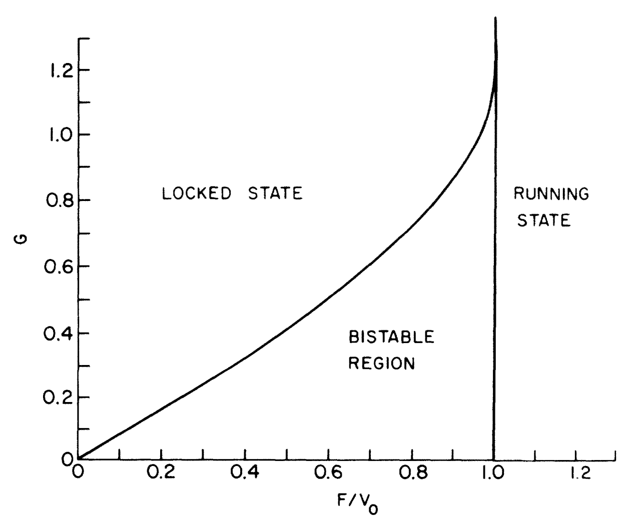

FIG. 3. Range of bistability in the tilted sinusoidal potential. $G = \gamma/(mV_0)^{1/2}$ is a dimensionless damping constant. This curve is parameter independent.

flux out of the well, to the right. In the extremely underdamped case, the escape is likely to be to the running state in which $\dot{\theta} > 0$.

Kramers's original work[1] discussed escape from a single initial well. In that case we have a relaxation process rather than steady-state transport. The relaxation process is, however, trivially related to a steady-state process,[11] if we add a source to the initial well replenishing the particles as they disappear, and if we similarly add a sink on the other side of the barrier. In all of these problems, for $E_b \gg kT$, equilibration within the lower and heavily populated portion of the well is rapid compared to equilibration involving crossing of the peak.[2] Therefore, the exact way the particles are introduced into the initial well does not matter. In our periodic case the particles escaping to the right out of a well, as in Fig. 1, will have come from a well to the left of the one under consideration. In the heavily damped case it will be from the adjacent left well. In a lightly damped case it can be from a far away well, via the running state of Fig. 2. In either case the source introduced to study the departure to the right will cancel the sink introduced for the study of arrival from the left, and we need not have any concern whether these fictitious sources and sinks introduce any approximations.

Our work results in a modest refinement of Kramers's original work[1] and of its subsequent application to Josephson junctions by Lee.[12] Our motivation for this modest extension is twofold. First of all it seems that Kramers's original discussion, for the case of extremely light damping, is still not fully appreciated. While, on the one hand, it has been elaborated and applied,[11–14] some of the most important and sophisticated treatments of noise-activated escape from the metastable state[15,16] do not reflect Kramers's understanding of the very lightly damped case. Biswas and Jha,[17] in the last paragraph of their paper, correctly allude to the point in question, but apparently without awareness of the extent to which Kramers had already given an answer. A paper by Matkowsky *et al.*[18] sets out to clarify Kramers's work, but for the nonmathematical reader Kramers's original discussion may be more accessible.

The second part of our motivation relates to the fact that Josephson-junction circuits with extremely low damping are of interest and have been studied.[19–21] Furthermore, thermal escape from metastable states in Josephson junctions has also been measured[19,20] and is of interest in connection with reliability questions in Josephson-junction logic.[21]

Kramers[1] discusses three separate approximations, depending on the degree of damping. The one that is most widely understood and appreciated applies to the heavily damped case, in which the particle exhibits highly diffusive behavior and the particle momentum relaxes to its thermal equilibrium distribution over a distance that is short compared with the scale of the potential variations. Specific application of this approximation to Josephson junctions with a small shunting capacitance was provided by Ambegaokar and Halperin.[22] An earlier discussion by Stratonovich[23] of externally synchronized electronic oscillators had treated the same set of equations and came to equivalent results. The Appendix to a recent paper[24] stresses the fact that a number of situations discussed in the modern literature require only very trivial extensions of Kramers's original discussion.

Kramers has a second result, his Eq. (25), which reduces to the above case, for heavy damping, but clearly extends to lower values of damping which we will call moderate damping. This result is

$$r=\frac{\omega_A}{2\pi|\omega_b|}\left[(\tfrac{1}{4}\eta^2+|\omega_b|^2)^{1/2}-\frac{\eta}{2}\right]e^{-E_b/kT}, \tag{1.3}$$

expressed as a probability of escape, per unit time, for particles in the initial well. Here

$$\omega_A=\omega_p(1-F^2/V_0^2)^{1/4}$$

is the frequency associated with particle motion in the bottom of the initial well. $\omega_p=(V_0/m)^{1/2}$ is the (plasma) frequency at $F=0$. ω_b is the analogous imaginary frequency associated with the unstable potential curvature at the barrier. (For the tilted sinusoid the absolute values of ω_A and ω_b are equal.) $\eta=\gamma/m$ is the momentum relaxation rate. The barrier height, as viewed from the bottom of the initial metastable valley, is given by

$$E_b=2V_0[(1-F^2/V_0^2)^{1/2}-(F/V_0)\arccos(F/V_0)]\ . \tag{1.4}$$

(From here on we take the origin of the energy scale so that the potential minimum under consideration is at $E=0$.) We assume throughout the paper that $kT \ll E_b$. For large η, Eq. (1.3) is approximated by

$$r=\frac{\omega_A|\omega_b|}{2\pi\eta}e^{-E_b/kT}\ . \tag{1.5}$$

This is the heavy damping limit discussed above. In the limit of small damping Eq. (1.3) is approximated by the result of the transition-state (ts) theory,

$$r_{\text{ts}}=\frac{\omega_A}{2\pi}e^{-E_b/kT}\ . \tag{1.6}$$

Equation (1.3) is also derived by Chandrasekhar.[15] In his Eq. (509) he claims this result is valid for all degrees of underdamping. We shall subsequently point out that that is incorrect. Note that Eq. (1.3) invokes the detailed shape of the initial potential valley only through its curvature at the initial minimum, and through the curvature at the barrier. The frequency at the initial minimum is inevitably involved. It is a measure of the phase space available there, and thus of the density which has to be depleted by the flux escaping across the barrier. The further details of the shape of the potential in the metastable valley do not enter Eq. (1.3), or its derivation. Indeed the derivations of this equation assume that particles crossing the barrier, followed back in time, or θ, well into the initial valley, have come from a region of θ which has a population which is in thermal equilibrium with the well bottom. Thus the derivations assume that the particle distribution, in most of the initial valley and within the energy ranges near the barrier peak, is undepleted from the value which represents thermal equilibrium with the valley minimum. The derivations only take into account the difficulty involved in crossing the barrier, and not the possibility that the population throughout this elevated energy range is depleted by the escape process taking place.

Kramers has a third set of approximations for the extremely underdamped case, which we shall subsequently discuss in more detail as a basis for our own refinement. It is clear that in the case of conservative motion, $\gamma=\eta=0$, a particle will remain at its initial energy permanently. Thus the particles which initially had enough energy to escape from the metastable well would do so, but would not be replaced by particles from lower-energy ranges, and there would be no escape at all from the initial valley except for a short initial transient. The rate at which particles can change energy depends on the damping and noise; both are proportional to γ. Thus, for very low damping, the energy changes occur very slowly, and the supply of particles up out of the bottom of the well cannot keep pace with the rate of escape for particles that have gained enough energy to cross the barrier. This leads to a depleted population in the energy range just above the barrier, and causes Eq. (1.3) to be incorrect. Kramers's third approximation treated this regime in which the particles diffuse upward along the energy or action coordinate and, not surprisingly, he found an escape rate proportional to η. This will be reviewed in detail in the next section. Kramers, thus, was aware that the bottleneck in escape from the initial well could be either the crossing time required for the barrier, as described by Eq. (1.3), or else could be the time required for thermal escape out of the bottom of the well. Kramers concluded, correctly, that the smaller of the rates, predicted by the two respective assumptions, would be the applicable escape rate. Our refinement is simply an attempt to treat the transition between the two cases more carefully, and to predict the departure from the simple proportionality between the escape rate and η, found for the highly underdamped case.

II. KRAMERS'S LOW-DAMPING LIMIT

In the case of very low η the particle is exposed to very little damping and very little noise and, as a result, follows the unperturbed conservative equations of motion for a long time. Thus we can classify particles, within the initial well, by their energy. The phase-space density will be almost constant along the dynamical path corresponding to a given energy. Alternatively we can classify paths by the action

$$I(E)=\oint p\,d\theta=m\oint\dot{\theta}\,d\theta\ , \tag{2.1}$$

which, within the well, will be a monotonic and continuous function of the energy. If $\rho(E)$ is the phase-space density at energy E, then ρdI gives the net population, or integrated distribution function, within the corresponding annular area in the phase plane. Kramers finds a flux, up along the I coordinate, given by

$$j_I=-\eta I(\rho+kT\partial\rho/\partial E)\ . \tag{2.2}$$

The first term in Eq. (2.2) is the relaxation due to damping, and describes a downward drift in energy toward the local minimum. The second term is a result of the fluctuations, and describes the diffusive process which permits particles to get away from the well minimum. In the absence of a current, $j_I=0$, and the resulting ρ describes thermal equilibrium

$$\rho_{eq}(E)=\rho_0 e^{-E/kT} . \quad (2.3)$$

The normalization constant ρ_0 is determined by the condition

$$\int \rho_{eq}(E)d\theta\, dp = N , \quad (2.4)$$

where N is the total number of particles in the valley, and this yields $\rho_0=\omega_A N/2\pi kT$.

To find an escape rate it is easiest to deal with a steady-state problem in which particles are continually fed into the bottom of the well, replacing those which escape at the top. The distribution function

$$\rho(E)=\beta(E)\rho_{eq}(E) , \quad (2.5)$$

then deviates from equilibrium by a correction factor β. By analogy to the heavily damped case[24] we can expect that the maintenance of the flux only requires appreciable deviations from equilibrium in those ranges of E where ρ_{eq} is relatively small. This will correspond to a β which is almost constant, except within a few kT of the barrier peak. For energies near the bottom of the well $\beta=1$, so that both $\rho_{eq}(E)$ and $\rho(E)$ obey the normalization condition Eq. (2.4). Furthermore, the relative distribution function, within the well, for the steady-state case will not differ seriously from that for the time-dependent case, in which the well population is depleted with time.

Substitution of Eq. (2.5) in Eq. (2.2) yields

$$j_I=-\eta I kT \rho_{eq}(E)\frac{\partial\beta}{\partial E} . \quad (2.6)$$

In the steady state j_I is independent of E. Integration from $E=E_1\cong kT$ to $E=E_b$ yields

$$j_I=\eta kT\frac{\beta(E_1)-\beta(E_b)}{\int_{E_1}^{E_b}(1/I)(1/\rho_0)e^{E/kT}dE} . \quad (2.7)$$

Let us first assume, as Kramers did, that the distribution function drops to zero at E_b, thus setting $\beta(E_b)=0$. The lower limit of the integral in Eq. (2.7) must be taken with care. Since $I\sim E$ in the quadratic potential at the bottom of the well, the integral will diverge if we take $E=0$ as a lower limit. From Eq. (2.6), it follows that for $E\ll kT$, the derivative $\partial\beta/\partial E\sim 1/E$. Thus the correction factor β, in the numerator of Eq. (2.7), grows like $\log(E/kT)$ at small energies. These two compensating divergencies in the fraction on the right-hand side (rhs) in Eq. (2.7) arise if we inject the current at the very bottom of the valley, where the phase space available for transport toward higher energies vanishes. If we avoid injection at the very bottom, then the Boltzmann factor becomes the dominant source of energy variation in the integrand, and the exact energy at which we inject is unimportant, as long as it is several kT below the barrier peak. With an equilibrium distribution in the bottom of the well, and if $\beta\rho_{eq}$ is still normalized as in Eq. (2.4), then $\beta(E_1)=1$. The fact that the integral in Eq. (2.7) is controlled by its upper integration limit yields

$$j_I=\eta I_b\rho_0 e^{-E_b/kT} . \quad (2.8)$$

Here $I_b=I(E_b)$ is the action of the path at the barrier peak. A particle on this path starts with zero velocity at the top of the barrier and, after an excursion into the metastable valley, returns again to the top of the barrier. The numerical evaluation of I_b as a function of the driving force F is shown in Fig. 4 adapted from Fig. 4 of Ref. 4. If F approaches V_0, which is a case of particular interest, the action can be given analytically. We find[4]

$$I_b=\tfrac{3}{10}I_0[2(1-F/V_0)]^{+5/4} , \quad (2.9)$$

where $I_0=16(mV_0)^{1/2}$ is the action at $F=0$. For subsequent reference we note that if $\beta(E_b)$ is taken as nonvanishing; then, instead of Eq. (2.8), we find

$$j_I=[1-\beta(E_b)]\eta I_b\rho_0 e^{-E_b/kT} . \quad (2.10)$$

From Eq. (2.8) and the normalization relation between ρ_0 and N we find an escape rate

$$r=j_I/N=(\eta I_b/kT)(\omega_A/2\pi)e^{-E_b/kT} . \quad (2.11)$$

Note the proportionality to η. For sufficiently large η, of course, Eq. (2.11) ceases to be applicable, and we must invoke Eq. (1.3) instead.

Our subsequent analytical discussion will continue to assume that injection does not occur at the very bottom of the well and that, therefore, the divergencies mentioned above are avoided. The Appendix discusses the modified results obtained for the escape rate if we insist that the injected particles really come from the well bottom. It will be shown, in the Appendix, that this correction is unimportant if $E_b\gg kT$.

III. REFINED TREATMENT FOR VERY WEAK DAMPING

We now continue to assume that the motion takes place along the energy coordinate, within the initial well, as described by Eq. (2.2), but will improve on Kramers's assumption that $\rho(E_b)=0$. For $E>E_b$ we will still allow a flux due to damping and fluctuations, as described by Eq. (2.2). Additionally, however, for $E>E_b$, we will allow an

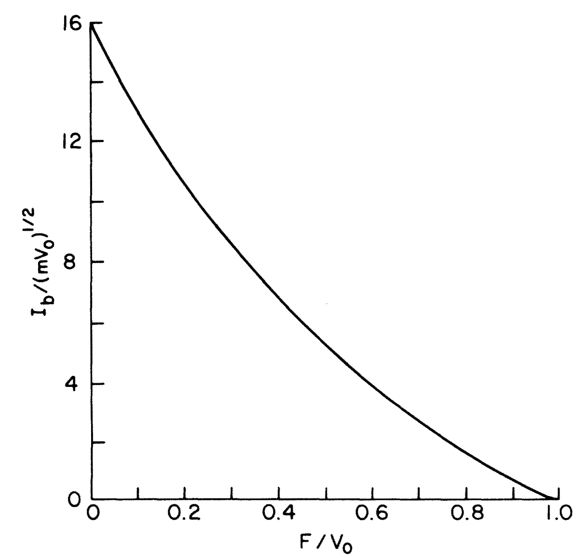

FIG. 4. Action as a function of F/V_0. At $F=0$ the action is $I_0=16(mV_0)^{1/2}$. This curve is parameter independent.

outflow from each energy range equaling the product of density and velocity at the location of the barrier (see Fig. 1). The phase-space density along a path of fixed energy will now be clearly nonuniform. The flux at the barrier peak, coming from the right into the well under consideration, will be zero. The fluctuations, offset by damping, will cause particles from lower-energy ranges to diffuse into the range in question, and thus the phase-space density builds up along the orbit in question reaching a maximum at the exit at $\theta=\theta_b$, for particles moving to the right. Thus β, defined as $\rho/\rho_{\rm eq}$, is no longer constant along a path of constant energy. Equation (2.6) still applies, however, with an effective $\beta(E)$ which must now describe the phase-space average occupation along a path of fixed energy, i.e., along a path which enters into the well and leaves it again. The density builds up along this path; thus the phase-space density at the exit port will be somewhat larger than that indicated by the phase-space average along the path. Let this additional correction factor be denoted by $\alpha>1$, but of order unity. The rate at which particles leave at the barrier peak, $\theta=\theta_b$, in the energy range dE will be

$$\rho(\theta_b)v\,dp=\rho\,dE=\alpha\beta(E)\rho_{\rm eq}(E)dE\ . \tag{3.1}$$

In the steady state this outflow must be compensated by a divergence in the vertical flow, with the vertical flow given by Eq. (2.6). Thus

$$\frac{dj_I}{dE}=-\alpha\beta\rho_{\rm eq}\ , \tag{3.2}$$

and after utilizing Eq. (2.6)

$$-\eta IkT\frac{\partial\rho_{\rm eq}}{\partial E}\frac{\partial\beta}{\partial E}-\eta IkT\rho_{\rm eq}\frac{\partial^2\beta}{\partial E^2}=-\alpha\beta\rho_{\rm eq}\ . \tag{3.3}$$

Dividing Eq. (3.3) by $\rho_{\rm eq}$, and using

$$\rho_{\rm eq}^{-1}(\partial\rho_{\rm eq}/\partial E)=-1/kT\ ,$$

we find

$$\eta IkT\frac{\partial^2\beta}{\partial E^2}-\eta I\frac{\partial\beta}{\partial E}-\alpha\beta=0\ . \tag{3.4}$$

We will be concerned with a relatively narrow energy range above $E=E_b$. In that range we will assume that I can be taken as sensibly constant, and equal to that at $E=E_b$. Then Eq. (3.4) becomes a linear homogeneous differential equation with constant coefficients, with solutions of the form $\beta=e^{sE/kT}$. Inserting this into Eq. (3.4) yields

$$(\eta I_b/kT)s^2-(\eta I_b/kT)s-\alpha=0\ , \tag{3.5}$$

or

$$s=\frac{1}{2}\left[1\pm\left[1+\frac{4\alpha kT}{\eta I_b}\right]^{1/2}\right]. \tag{3.6}$$

The solution in Eq. (3.6) with the + sign gives a positive s and a density increasing exponentially with energy. It is clearly not relevant. Thus

$$s=-\frac{1}{2}\left[\left[1+\frac{4\alpha kT}{\eta I_b}\right]^{1/2}-1\right], \tag{3.7}$$

and $e^{sE/kT}$ accentuates the dropoff with energy present in equilibrium. s, as given by Eq. (3.7), is a function only of $\alpha kT/\eta I_b$. The factor α is of order unity. ηI_b is the energy loss, due to damping, in one cycle of the motion, e.g., from departure at the barrier peak until the subsequent return. Thus $kT/\eta I_b$ is smaller or larger than unity, depending on whether the particle loses more or less than kT in the round trip through the metastable well. For severely underdamped systems, $kT/\eta I_b\gg 1$ and $s\sim-(\alpha kT/\eta I_b)^{1/2}$. Thus $\rho\sim\rho_{\rm eq}e^{sE/kT}$ and decreases *much* faster with increasing energy than $\rho_{\rm eq}$, thereby invalidating the reasoning leading to Eq. (1.3).

There is an alternative way of viewing this severely underdamped case closely related to the discussions in Refs. 1 and 11. As we have pointed out, Eq. (1.3) essentially gives the rate at which particles move across the barrier, taking as the source a thermal equilibrium population in the metastable well. In thermal equilibrium, however, if $kT\gg\eta I_b$, then particles entering the metastable well from the right, with a kinetic energy of the order of kT at the barrier peak, are likely to bounce out of the well again. Thus a high proportion of the thermal equilibrium flux out of the metastable well consists of particles which entered the well, and were reflected, rather than particles boiling up out of the well. Only a small proportion of the emerging flux consists of the latter. If, therefore, the particles entering the metastable valley from the right are absent, then the escaping particle flux must be much smaller than that given by Eq. (1.3). In the alternative limit, $\eta I_b\gg kT$, the correction factor $e^{sE/kT}$ becomes unimportant.

To complete our calculation we must now match the probability density specified by Eq. (3.7), for $E>E_b$, to a solution of Eqs. (2.6) and (2.7) for $E<E_b$. We require continuity of β, and of $\partial\beta/\partial E$, or alternatively of β and of j_I, at $E=E_b$. Equation (2.10) can be rewritten, with the use of $\rho_0=\omega_A N/2\pi kT$, as

$$j_I=[1-\beta(E_b)](\eta I_b/kT)(\omega_A N/2\pi)e^{-E_b/kT}\ . \tag{3.8}$$

For $E\geq E_b$ we assume

$$\beta(E)=\beta(E_b)\exp[s(E-E_b)/kT]\ ,$$

so that $\beta(E)$ is continuous at $E=E_b$. Using $\rho=\beta(E)\rho_0e^{-E_b/kT}$, we find from Eq. (2.6) a current

$$j_I=-s\beta(E_b)(\eta I_b/kT)(\omega_A N/2\pi)\times\exp[s(E-E_b)/kT-E/kT] \tag{3.9}$$

for $E\geq E_b$. Equating the two rhs expressions in Eqs. (3.8) and (3.9), at $E=E_b$, gives $1-\beta=-s\beta$ or

$$\beta(E_b)=1/(1-s)\ . \tag{3.10}$$

Substituting this in Eq. (3.8) yields

$$r=j_I/N=\frac{[1+(4\alpha kT/\eta I_b)]^{1/2}-1}{[1+(4\alpha kT/\eta I_b)]^{1/2}+1}\left[\frac{\eta I_b}{kT}\right]\frac{\omega_A}{2\pi}e^{-E_b/kT}\ . \tag{3.11}$$

As η tends to zero this result reduces to Eq. (2.11). As η tends to infinity Eq. (3.11) yields $r=\alpha r_{\rm ts}$, where $r_{\rm ts}$ is given by Eq. (1.6).

In Fig. 5 we have plotted the various theoretical results. Escape rates are measured in units of the transition-state

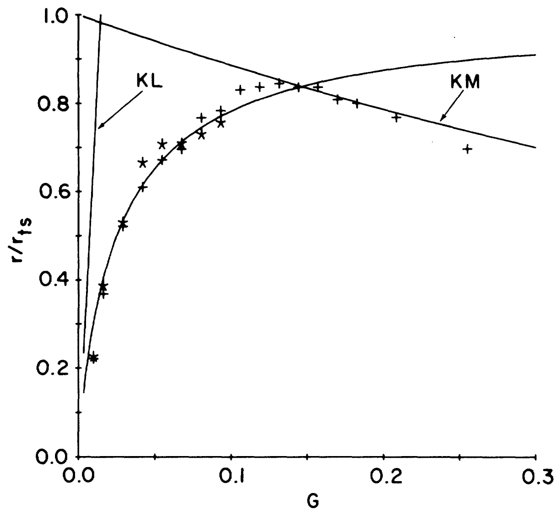

FIG. 5. Escape rate, in units of the transition-state theory result, as a function of the dimensionless damping constant G for $F/V_0=0.985$ and $E_b/kT=3.938$. The solid lines are Kramers's moderate-damping result (KM), Kramers's low-damping result (KL), and our new refined low-damping result, Eq. (3.11), for $\alpha=1$. These theoretical results are compared with the results of a conventional computer simulation of escape events (+) and also with the results of a faster method (∗) simulating the motion of the particle only near the energy of the barrier peak. The faster method is valid only for low damping.

theory result, Eq. (1.6), and are shown as a function of the dimensionless damping constant $G=\gamma/(mV_0)^{1/2}$. The curve labeled KM is Kramers's moderate-damping result, Eq. (1.3), divided by r_{ts}. The curve labeled KL is Kramers's low-damping result, Eq. (2.11), in units of r_{ts}. The third curve shown is our result, Eq. (3.11), for $\alpha=1$. Actually, of course, we would have expected $\alpha>1$, as already discussed. Our best fit, however, was obtained for $\alpha=1$. Thus α was used as an adjustable parameter, though not a parameter with a great range of variability. The curves shown in Fig. 5 are for a field $F/V_0=0.985$ and $V_0/kT=1135.9$ corresponding to a ratio $E_b/kT=3.938$. These values describe a Josephson-junction circuit with a critical current of 0.2 mA, a bias current of 0.197 mA, and a capacitance of 1 pF at a temperature of 4.2 K. A shunt resistance of 100 Ω corresponds to a dimensionless damping constant $G=0.012\,83$. For such a junction our result, Eq. (3.11), predicts a lower escape rate than the results of Kramers, and we expect that over this range of damping constants our result is a better approximation of the escape rate. To check this prediction, we have performed computer simulations which we will discuss in the next section.

IV. COMPUTATIONAL RESULTS

With the use of a dimensionless time $\tau=\omega_p t$, where $\omega_p=(V_0/m)^{1/2}$ is the plasma frequency at $F=0$, the Langevin equation (1.1) reduces to

$$\frac{d^2\theta}{d\tau^2}+G\frac{d\theta}{d\tau}=-\sin\theta+\frac{F}{V_0}+\frac{\xi}{V_0} \tag{4.1}$$

and

$$\langle[\xi(\tau)/V_0][\xi(\tau')/V_0]\rangle=(2\gamma kT/V_0^2\omega_p)\delta(\tau-\tau') . \tag{4.2}$$

Here $G=\gamma\omega_p/V_0=\gamma/(mV_0)^{1/2}$ is the dimensionless damping constant. Integrating Eq. (4.1) over a small time interval $\Delta\tau$ yields

$$\theta_{n+1}=2\theta_n-G(\theta_n-\theta_{n-1})\Delta\tau +(F/V_0-\sin\theta_n+\hat{\xi}_n/V_0)(\Delta\tau)^2 . \tag{4.3}$$

$\hat{\xi}_n$ is a new stochastic process defined by

$$\hat{\xi}_n=\frac{1}{\Delta\tau}\int_{n\Delta\tau}^{(n+1)\Delta\tau}\xi(\tau)d\tau , \tag{4.4}$$

and it has the property

$$\langle\hat{\xi}_n\hat{\xi}_m/V_0^2\rangle=2(GkT/V_0\Delta\tau)\delta_{nm} . \tag{4.5}$$

To check the accuracy of the difference equation (4.3), we have also used an integration scheme, developed by Morf and Stoll,[25] which is accurate to higher powers of $\Delta\tau$ than Eq. (4.3). The two methods gave identical results for integration steps $\Delta\tau\leq 0.03$. We have approximated the noise $\hat{\xi}_n$ with pseudorandom numbers q_n distributed uniformly in the interval $(-0.5,0.5)$. Since $\langle q_n q_m\rangle=\frac{1}{12}\delta_{nm}$, we have used a random force $\hat{\xi}_n=\epsilon q_n$ in Eq. (4.3) with $\epsilon=(24GkT/V_0\Delta\tau)^{1/2}$.

In a conventional simulation of escape events we start with the particle at the bottom of the well and follow the particle until it escapes over the barrier, measuring the time it takes the particle to escape and to travel some distance away from the barrier peak in the direction of increasing θ. The results of the conventional calculation are shown in Fig. 5 (data points indicated by +). Each data point represents an average of 500 escape events. The random generator was started at the same point (seed) for each data point. For $G=0.205\,28$, six data points have been calculated, each with a different seed. We found an average escape rate of $r/r_{ts}=0.74$ and a variance of 0.05. In most of the literature escape rates are plotted on a logarithmic scale; in that case, the alternative prefactors discussed in our paper would be barely distinguishable.

In principle we should compare these numerical results with analytical results taking into account that the particles are injected at the very bottom of the valley. However, as shown in the Appendix, as well as in a simulation where we injected particles at energies above the bottom of the well, the escape rate is not sensitive to the precise injection mechanism. In this particular alternative simulation we invoke an equilibrium distribution ρ_{eq} for energies below the energy of the injected particles. At the injection energy the distribution function is continuous, but $d\rho/dE$ is discontinuous by an amount corresponding to the injected current. Within the accuracy of our calculation the escape rate remains the same, until the injection energy comes within kT of the barrier energy. The alternative simulation just discussed, corresponding to an actual physical injection process at an energy above the well bottom, is distinct from a method, to be discussed subsequently, for handling the numerical simulation for escape out of the well.

In the conventional simulation the particle spends most of the time near the bottom of the well. Most of the computing power is used to simulate the behavior of the particle in a region of the phase space which can easily be treated analytically by solving the Langevin equation (1.1) or the associated Fokker-Planck equation. It is, therefore, desirable to have a method which uses the computer only to simulate the behavior of the particle in an energy range close to the barrier peak energy. For Hamiltonian systems, such computational methods have been introduced by Bennett.[26] We will now present an adaption of Bennett's ideas to our dissipative problem.

To keep the particle away from the bottom of the well, we introduce a reflecting bottom at an energy E_- (see Fig. 6). We inject the particles at this energy with a rate j. Each time the energy of the particle falls below E_-, the particle is restarted at this energy. The motion of the particle is simulated until it eventually escapes over the barrier. We register the total dwell time τ_d of the particle in a small energy range (E_+,E_-) with a width $\Delta E = E_+ - E_- \ll kT$. The dwell time in turn yields the number of particles in this energy range

$$j\tau_d = \int \rho dI \cong \rho(E_-)\Delta I = \beta(E_-)\rho_{eq}(E_-)\Delta I \ , \tag{4.6}$$

where we have used Eq. (2.5) and $\Delta I = I_+ - I_-$ with $I_\pm = I(E_\pm)$. We now match the density $\rho(E_-)$ in the interval to Kramers's solution Eq. (2.7) for energies $E < E_-$. In this calculation, where E_- is only a demarcation between simulation and analytic treatment, rather than a physically significant energy, we require continuity for ρ *and* for $d\rho/dE$ at E_-. The injection of particles at the energy E_- is an artifice for calculational purposes only and not a real source of particles. The injection current simply provides for the continuity of current. Without injection, and with a reflecting barrier, we would otherwise have a vanishing upward flux, just above the reflecting barrier. From Eq. (2.7) with E_- as the upper integration limit, we find

$$\beta(E_-) = 1 - (j/\eta I_- \rho_0)e^{E_-/kT} \ . \tag{4.7}$$

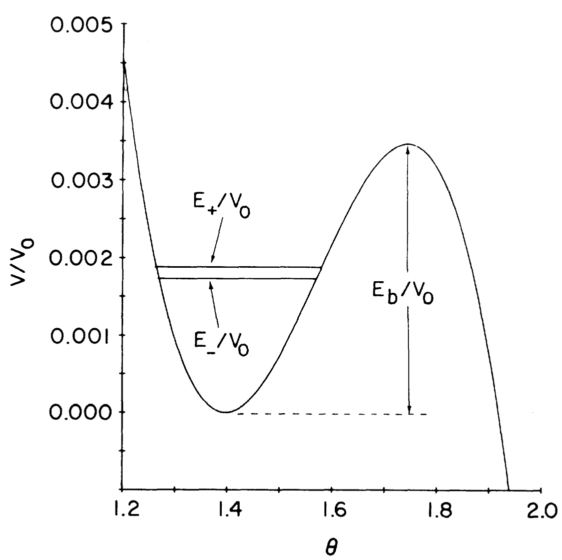

FIG. 6. Same potential as in Fig. 1 but for $F=0.985V_0$. To speed up the calculation, we have introduced a reflecting bottom at the energy E_-, and we calculate the average dwell time of particles in the small energy range (E_+,E_-).

Using Eq. (4.7) to eliminate β in Eq. (4.6) and solving for j yields a rate

$$r = \frac{j}{N} = \frac{\Delta I}{kT\tau_d}\beta(E_-)\frac{\omega_A}{2\pi}e^{-E_-/kT} \ , \tag{4.8}$$

with $\beta(E_-) = 1/(1+\Delta I/\eta I_- \tau_d)$. If our energy interval is not too close to the barrier peak $\beta(E_-) \cong 1$. Equation (4.8) relates the dwell time τ_d to the escape rate. The time for simulation of an escape event is proportional to $e^{E_b/kT}$ for the conventional method and proportional to $\exp[(E_b - E_-)/kT]$ for the second method. Thus the second method is considerably faster. The disadvantage of this second method is that there are two additional parameters, E_- and ΔE, against which one has to test numerical stability. The results of this second calculation are also shown in Fig. 5 (data points shown as $*$). Again all data shown has been obtained for the same seed. To estimate the accuracy for our alternative method we have calculated data points for six different random-number generation seeds at $G = 0.051\,31$. We obtained an average escape rate $r/r_{ts} = 0.68$ with a variance of 0.06. With increasing G the variance increases rapidly. It is seen that, for small damping constants G, we obtain excellent agreement both with the conventional method and with our new result, Eq. (3.11).

APPENDIX: PARTICLE INJECTION FROM WELL MINIMUM

If injection occurs at the very bottom of the well where the available phase space for transport disappears, then β must diverge as $E \to 0$, as already pointed out after Eq. (2.7). Thus there is an extra bump in the population near the bottom of the well. The relationship between j_I and ρ at higher energies, as discussed in Sec. III, will be unaffected. The proper value of N, however, used in Eq. (3.11), expressing the total well population which is being depleted by j_I, will increase. We show here that for $E_b \gg kT$, this is not a significant increase, despite the divergence in the phase-space density. Equation (2.6) yields

$$\frac{\partial \beta}{\partial E} = -\frac{j_I}{\eta I kT \rho_{eq}} \ . \tag{A1}$$

For a harmonic oscillator, and therefore near the bottom of our well, $I = 2\pi E/\omega_A$. Thus Eq. (A1) becomes

$$\frac{\partial \beta}{\partial E} = -\frac{j_I \omega_A}{2\pi\eta kT\rho_0 E e^{-E/kT}} \ . \tag{A2}$$

The rhs denominator of (A2) depends on E through the term $Ee^{-E/kT}$. This has a maximum at $E = kT$, and above that it is dominated by the variation of the exponential, and below that by the linear factor resulting from the phase-space density. As a crude approximation we replace $e^{-E/kT}$ by unity, for $E < kT$. For $E > kT$ the diminishing phase-space density is unimportant, and $\beta = 1$ to a very good approximation, until E becomes large enough to approach the barrier peak. Integrating this modified form of Eq. (A2), and requiring β to be unity at $E = kT$ (to determine the constant of integration) gives $\beta = 1 + \delta\beta$, where

$$\delta\beta = -(j_I\omega_A/2\pi\eta kT\rho_0)\ln(E/kT) \ . \tag{A3}$$

$\delta\beta$ is the source of the extra population, i.e., the source of the change δN in N, that we have to take into account in the modified form of Eq. (3.11). Therefore, the increase in population is

$$\delta N = \int_{E<kT} \delta\beta \rho_{eq} dI \ . \tag{A4}$$

Again, for our rough estimate, we take $\rho_{eq}=\rho_0$ in Eq. (A4). Thus

$$\delta N = -\frac{j_I \omega_A}{2\pi\eta kT} \int_0^{kT} \ln\left[\frac{E}{kT}\right] d\left[\frac{2\pi E}{\omega_A}\right] , \tag{A5}$$

where we have used $I=2\pi E/\omega_A$, valid for a harmonic oscillator. Integration of Eq. (A5) gives $\delta N = j_I/\eta$. Let the original value of N, which did not allow for the low-energy divergence, be denoted by N_0, and the corresponding escape rate in Eq. (3.11) by r_0. The low-energy divergence, therefore, diminishes the result given in Eq. (3.11) by a factor

$$\frac{N_0}{N_0+\delta N} = \frac{j_I/r_0}{j_I/r_0+j_I/\eta} = \frac{1}{1+(r_0/\eta)} \ . \tag{A6}$$

Figure 5 shows that r_0 varies linearly with η, for small η, and r_0 reaches a maximum for larger η. Thus r_0/η is largest at small η, and this is where the reduction factor of Eq. (A6) becomes most significant. From Eq. (2.11) we find

$$r_0/\eta = (\omega_A I_b / 2\pi kT) e^{-E_b/kT} \ . \tag{A7}$$

The linearity between I and E which holds for a harmonic oscillator, does not apply at the barrier, but as an order-of-magnitude estimate we can still take $I_b = 2\pi E_b/\omega_A$. Thus (A7) becomes

$$r_0/\eta = (E_b/kT) e^{-E_b/kT} \ . \tag{A8}$$

For $E_b \gg kT$ we therefore find $r_0/\eta \ll 1$, and the correction factor of Eq. (A6) remains close to unity.

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