Escape-field distribution for escape from a metastable potential well subject to a steadily increasing bias field

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The first two moments of the escape-field distribution are evaluated for a particle in a steadily ramped potential. Implications for macroscopic quantum tunneling are discussed.

If a system with a one-dimensional degree of freedom x, described by a potential $V(x)$ of the general shape drawn in Fig. 1, is initially prepared in a suitable state or distribution in the potential well, it will escape out of this well, either by thermal activation over the barrier at high temperatures, or by quantum tunneling at low temperatures. If in addition, the potential includes a term $-Fx$, where F is a bias field which can be experimentally varied, then a convenient way to study the escape process is to steadily ramp up the field and monitor the value of F at which escape occurs. Since the escape process is stochastic, the escape field will differ from run to run of the experiment, and one must consider the entire distribution $P(F)$ of escape fields.

The above procedure seems to have been first used to study thermal phase-slip events in current or flux-biased Josephson junctions and superconducting quantum interference devices.[1-3] These systems were later studied[4,5] at lower temperatures with a view to seeing macroscopic quantum tunneling (MQT).[6] In these systems, the distribution $P(F)$ can be very well sampled, and following Ref. 3, the data can be converted directly into an F-dependent escape rate $\Gamma(F)$. Recently, Giordano and co-workers have examined[7] the depinning of a magnetic domain wall in very thin Ni wires subject to a biasing magnetic field as another candidate system for MQT. Sampling the distribution appears to be harder in this system, and only the mean escape field has been measured yet.

The purpose of this short and technical note is to find analytic formulas for the mean and width of the escape-field distribution, in the hope that these will be useful in analyzing experiments such as those of Ref. 7, when the full $P(F)$ cannot be studied, and only its mean and width can be adequately measured. The essential dependence on temperature and parameters of the potential have previously been found semiempirically by Kurkijärvi[1,8] when the escape is by overdamped thermal activation. It nevertheless seems worthwhile to present our analysis as it refines and gives a firm basis to Kukijärvi's answers, and can be extended to the cases when the escape is by quantum tunneling or by thermal activation with moderate damping.

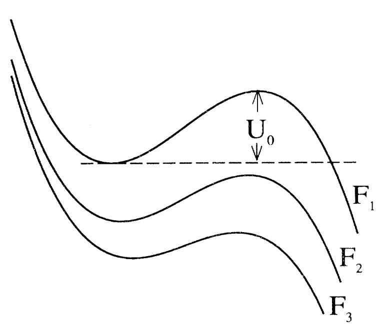

FIG. 1. Metastable potential wells for three different bias fields, $F_3 > F_2 > F_1$. The curves are displaced vertically for clarity. The barrier height U_0 is shown for $F=F_1$.

The escape-field distribution is related to $\Gamma(F)$ by the following argument.[1,3] Let the field $F=0$ at time $t=0$,[9] and let it be ramped up at a steady rate $\dot{F}$. The probability $W(F(t))$ that the system will *persist* in the metastable state up to time t is given by

$$W(F(t))=\exp\left[-\int_0^t \Gamma(F(t'))dt'\right] . \tag{1}$$

Changing the variable of integration from t' to $F(t')$, we have

$$P(F)=-\frac{d}{dF}W(F)=\frac{\Gamma(F)}{\dot{F}}\exp\left[-\int_0^F \frac{\Gamma(F')}{\dot{F}}dF'\right] . \tag{2}$$

We shall refer to Eq. (2) as the Kurkijärvi-Fulton-Dunkelberger (KFD) formula.[10] Note that $P(F)\to 0$ as $F\to 0$ because of the pre-exponential factor $\Gamma(F)$, and also as $F\to F_c$ because of the exponential factor.

Since escape (quantum or thermal) is improbable if the potential barrier is large, we focus on values of F close to the critical field F_c at which the barrier disappears completely. It is then a good approximation to use a cubic potential for $V(x)$, in which case, the barrier height $U_0(F)$ and the small oscillation frequency $\omega(F)$ are given by[1]

$$U_0(F)=U_c\epsilon^{3/2} , \tag{3}$$

$$\omega(F)=\omega_c\epsilon^{1/4} , \tag{4}$$

where U_c and ω_c are characteristic parameters of the unbiased potential, and

$$\epsilon=1-F/F_c \tag{5}$$

is a reduced bias field. We shall only examine cases where the escape rate can be written as

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$$\Gamma(\epsilon)=A\epsilon^{a+b-1}\exp(-B\epsilon^{b}) \ . \tag{6}$$

This form is broad enough to cover a large variety of interesting cases. The quantities A, B, a, and b depend on whether the escape is quantal or thermal, and the degree and type of damping. In Table I, we give illustrative formulas for various cases involving Ohmic damping, by which we mean that the classical equation of motion for x includes a frictional force $-\eta\dot{x}$, with the "mass" taken as unity. The results for thermal activation are from the celebrated paper by Kramers,[11] and those for quantum tunneling from Refs. 6 and 12. It should be noted that the most important feature of Γ is the exponent, so our results should hold to good approximation even when the prefactor has corrections (possibly ϵ dependent) or a somewhat different form.[13] We refer the reader to Ref. 14 for a comprehensive discussion of these points, and of the domain of validity of the formulas in Table I.

We find that for small ramp rates, the mean $\langle\epsilon\rangle$ and the variance σ_ϵ^2 (which are trivially related to $\langle F\rangle$ and σ_F^2) are given asymptotically by

$$\langle\epsilon\rangle=\left[\frac{\ln X}{B}\right]^{1/b}\left[1+\frac{1}{b\ln X}\left[\frac{a}{b}\ln\ln X+\gamma\right]+\cdots\right] , \tag{7}$$

$$\sigma_\epsilon^2=\frac{(\ln X)^{-2+2/b}}{B^{2/b}}\left[\frac{\pi^2}{6b^2}+\frac{1}{b^3\ln X}\{2a[\bar{v}^2+\bar{v}+\pi^2/6]-(b-1)[\pi^2\bar{v}^2/3-\psi''(1)]\}+\cdots\right] , \tag{8}$$

$$\bar{v}=\frac{a}{b}\ln\ln X+\gamma , \tag{9}$$

where $\gamma=0.5772\ldots$ is the Euler-Mascheroni constant, $\psi''(1)=-2.404\ldots$ is a particular value of the tetragamma function,[15] and

$$X=\frac{F_c}{\dot{F}}\frac{A}{bB^{1+a/b}} \ . \tag{10}$$

The details are given in the Appendix.[16] The ramp rate $\dot{F}$ must clearly be small, as otherwise the system will not be able to maintain an equilibrium form in the initial state. A proper criterion for how small $\dot{F}$ must be will be obtained below, but we note here that in the experiments, X is often as large as 10^6, and even larger values may be desirable as the true expansion parameter in Eqs. (7) and (8) is $1/\ln X$. For thermally activated escape with large damping—the case considered in Ref. 1—$a=0$, $b=3/2$, the X's in Eq. (10) above and Eq. (11) in Ref. 1 are identical, and our answers for $\langle\epsilon\rangle$ and σ_ϵ agree precisely with the numerical results of Ref. 1 for $X\geq 10$ and $X\geq 10^3$, respectively. For $X=10$, our result for σ_ϵ is alternately too small or too large by about 10%, depending on whether the correction to the leading term is or is not included. This comparison gives some measure of the importance of the correction terms and the range of X over which the expansions (7) and (8) can be trusted.

Let us now see how small $\dot{F}$ must be. The validity of Eq. (6) for the escape rate (either thermal or quantal) requires $B\epsilon^b \gg 1$. The maximum of the KFD distribution should clearly be located inside this region of validity. This maximum is found by solving the equation $d\ln\Gamma/d\epsilon=\Gamma/\dot{\epsilon}$, which can be reduced to

$$X=\frac{\exp(B\epsilon^b)}{(B\epsilon^b)^{a/b}} \ . \tag{11}$$

Taking $B\epsilon^b\geq 15$ as an operational criterion, we obtain $X\gtrsim O(10^6)$ for all cases listed in Table I. For both the Josephson-junction-based and magnetic MQT candidate systems, one has $\omega_c/2\pi\sim 1$ GHz, which combined with $X\gtrsim 10^6$ yields $\Gamma\lesssim 10^4\ \mathrm{sec}^{-1}$, and $|\dot{\epsilon}|\lesssim 10^2\ \mathrm{sec}^{-1}$.

In summary, we have found [Eqs. (7) and (8)] the mean and width of the escape-field distribution. As discussed in Ref. 5, a convincing demonstration that one is observing MQT requires measuring the parameters U_c, ω_c, and F_c accurately. The last quantity must be measured to particularly high precision. This is best done at high temperatures when the escape is thermally activated. In that regime, Eqs. (7) and (8) show, as expected, that the dominant behavior is governed by the exponent B in the rate, the prefactor A being much less important. A plot

TABLE I. Parameters of the thermal and quantal escape rate for various degrees of Ohmic damping. See Refs. 6 and 11–14 for a discussion of corrections and domain of validity of the various limits.

Escape mechanism	Damping	A	B	a	b
Thermal	Low	$18\eta U_c/5\pi k_B T$	$U_c/k_B T$	1	3/2
Thermal	Moderate	$\omega_c/2\pi$	$U_c/k_B T$	$-1/4$	3/2
Thermal	High	$\omega_c^2/2\pi\eta$	$U_c/k_B T$	0	3/2
Quantal	None	$(216 U_c\omega_c/\pi\hbar)^{1/2}$	$36U_c/5\hbar\omega_c$	5/8	5/4
Quantal	High	$(3U_c\eta^7/\hbar\omega_c^6)^{1/2}$	$3\pi\eta U_c/\hbar\omega_c^2$	0	1

of $\langle F \rangle$ versus σ_F should therefore essentially be a straight line with y intercept F_c and a very weakly temperature-dependent slope $2\pi/(3\sqrt{6}\ln X)$. This approach may provide another means of determining F_c and $\ln X$ and thus at least some of the system parameters.

Note added in proof. After submitting this paper, the author learned of an approximately similar analysis[18] for the case of thermal escape, and of extensive measurements[19] of the escape-field distribution for magnetization reversal in small particles. I thank B. Barbara and W. Wernsdorfer for this information.

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APPENDIX

The controlling factor in the integrals for $\langle F \rangle$ and $\langle F^2 \rangle$ is clearly the exponent $s(F)$ [or equivalently $s(\epsilon)$] in the persistence probability $W(F)$. It is therefore desirable to make a change of variables from ϵ to s. This would be quite straightforward if a vanished, and the analysis that follows is tedious largely because this is not so.

The first step is therefore to write ϵ as a function of s. We have

$$s(\epsilon)=\int_0^F \frac{\Gamma(F')}{\dot{F}}dF=\frac{1}{|\dot{\epsilon}|}\int_\epsilon^\infty \Gamma(\epsilon')d\epsilon' . \tag{A1}$$

Repeated integration by parts gives

$$s(\epsilon)=\frac{A\epsilon^a}{bB|\dot{\epsilon}|}e^{-B\epsilon^b}\left[1+\frac{a}{bB}\epsilon^{-b}+\frac{a(a-b)}{b^2B^2}\epsilon^{-2b}+\cdots\right] . \tag{A2}$$

Defining $q=B\epsilon^b$, and taking logs, we get after a little rearrangement,

$$q=Z+\frac{a}{b}\ln q+\frac{a}{b}\frac{1}{q}+\frac{a(a-2b)}{2b^2}\frac{1}{q^2}+O(q^{-3}) , \tag{A3}$$

where

$$Z=\ln\frac{A}{bB^{1+a/b}|\dot{\epsilon}|s}=\ln(X/s) . \tag{A4}$$

The important values of s are around unity, so we will solve Eq. (A3) for q when $Z \gg 1$. This can be done as an expansion in powers of $1/Z$ and $(\ln Z)/Z$, and we get

$$q \approx Z+\frac{a}{b}\ln Z+\frac{a}{bZ}\left[\frac{a}{b}\ln Z+1\right] -\frac{a}{2bZ^2}\left[\frac{a^2}{b^2}\ln^2 Z+2\frac{a}{b}\left[1-\frac{a}{b}\right]\ln Z+\left[2-3\frac{a}{b}\right]\right] +O(Z^{-1}\ln Z)^3 . \tag{A5}$$

This is almost in the desired form, and raising it to the $1/b$th power would give us ϵ, but let us first make the s dependence explicit, treating s formally as a quantity of order unity. Writing $Z_0=\ln X$, we have

$$q\approx Z_0+\frac{a}{b}\ln Z_0-\ln s+\frac{a}{bZ_0}\left[\frac{a}{b}\ln Z_0-\ln s+1\right] -\frac{a}{2bZ_0^2}\left[\frac{a^2}{b^2}\ln^2 Z_0+2\frac{a}{b}\left[1-\frac{a}{b}\right]\ln Z_0+\left[2-3\frac{a}{b}\right]\right] -\frac{a}{2bZ_0^2}\ln^2 s+\frac{a}{bZ_0^2}\left[\frac{a}{b}\ln Z_0-\frac{a}{b}+1\right]+\cdots . \tag{A6}$$

It pays to introduce the combination

$$v(s)=\frac{a}{b}\ln Z_0-\ln s , \tag{A7}$$

in terms of which we can rewrite Eq. (A6) as

$$q\approx Z_0+v+\frac{a}{bZ_0}(v+1) -\frac{a}{2bZ_0^2}[v^2+2(1-a/b)v+(2-3a/b)]+\cdots . \tag{A8}$$

To evaluate $\langle \epsilon \rangle$ and $\langle \epsilon^2 \rangle$ we need $q^{1/b}$ and $q^{2/b}$. For a general exponent r, one more expansion gives

$$q^r\approx Z_0^r+rZ_0^{r-1}\left[v+\frac{a}{bZ_0}(v+1)-\frac{a}{2bZ_0^2}[v^2+2(1-a/b)v+(2-3a/b)]\right] +\frac{r(r-1)}{2}Z_0^{r-2}\left[v^2+\frac{2a}{bZ_0}(v^2+v)\right]+\frac{r(r-1)(r-2)}{6}Z_0^{r-3}+\cdots . \tag{A9}$$

The second step is to rewrite $\langle \epsilon^n \rangle$ as an integral over s. We have

$$\langle \epsilon^n \rangle=\int_0^\infty \epsilon^n \frac{dW}{d\epsilon}d\epsilon=B^{-n/b}\int_{\epsilon=0}^{\epsilon=\infty} q^{n/b}(s)(de^{-s}) . \tag{A10}$$

Substituting Eq. (6) in Eq. (A1) we get $s(\infty)=0$, and $s(0)=e^{Z_0}\Gamma(1+a/b)\gg 1$. The error made by replacing the lower limit in the integral (A10) by $s=\infty$ is of order $e^{-s(0)}\sim e^{-X}$, which is clearly negligible. Thus,

$$\langle \epsilon^n \rangle=B^{-n/b}\int_0^\infty q^{n/b}(s)e^{-s}ds . \tag{A11}$$

The final step is to substitute Eq. (A9) in (A11) and evaluate the integrals. Regarding e^{-s} as a distribution for s, and writing $\overline{v^n} \equiv \langle v^n \rangle$, we obtain[17]

$$\bar{v} = \frac{a}{b}\ln Z_0 + \gamma \; , \tag{A12}$$

$$\overline{v^2} = \bar{v}^2 + \frac{\pi^2}{6} \; , \tag{A13}$$

$$\overline{v^3} = \bar{v}^3 + \frac{\pi^2}{2}\bar{v} - \psi''(1) \; . \tag{A14}$$

Using these, we obtain

$$\langle q^r \rangle = Z_0^r \left[1 + \sum_{j=1} Z_0^{-j} f_j(r, Z_0) \right] , \tag{A15}$$

where

$$f_1 = r\bar{v} \; , \tag{A16}$$

$$f_2 = r\frac{a}{b}(\bar{v}+1) + \frac{r(r-1)}{2}\left[\bar{v}^2 + \frac{\pi^2}{6} \right] , \tag{A17}$$

$$\begin{aligned} f_3 = & -r\frac{a}{2b}\left[\bar{v}^2 + 2(1-a/b)\bar{v} + \frac{\pi^2}{6} + 2 - 3\frac{a}{b} \right] \\ & + r(r-1)\frac{a}{b}\left[\bar{v}^2 + \bar{v} + \frac{\pi^2}{6} \right] \\ & + \frac{r(r-1)(r-2)}{6}\left[\bar{v}^3 + \frac{\pi^2}{2}\bar{v} - \psi''(1) \right] . \end{aligned} \tag{A18}$$

Putting $r = 1/b$, multiplying by $B^{-1/b}$, and recalling that $Z_0 = \ln X$, we obtain Eq. (7) of the text. Likewise, putting $r = 2/b$ gives $\langle q^{2/b} \rangle$, and Eq. (8) follows from $B^{2/b}\sigma_\epsilon^2 = \langle q^{2/b} \rangle - \langle q^{1/b} \rangle^2$.

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[9]We assume that escape is extremely improbable when $F=0$, i.e., that we can take $\Gamma(F=0)=0$. If not, we simply replace the lower limit $F=0$ in Eq. (2) by some other suitable choice.

[10]The KFD formula can be written in several equivalent ways. The form (2) makes it apparent that $\Gamma(F) = -\dot{F}(d/dF)\ln\int_F^\infty P(F')dF'$, the argument of the logarithm being identical to $W(F)$. If $P(F)$ is measured in the form of a histogram, the simplest discrete difference approximation to the derivative in the above equation immediately leads to and vindicates the commonly used approximation (7) of Ref. 3, which is there justified by arguing that $\int_F^\infty P(F')dF'$ should be fit by a series of exponentials rather than straight lines between adjacent bins.

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[16]The expansion for $\langle \epsilon \rangle$ is in fact found up to relative order $O(\ln\ln X/\ln X)^3$, but the higher order terms are unlikely to be useful in themselves. They are needed to find σ_ϵ^2.

[17]The required integrals are of the first three powers of $\ln s$ weighted by e^{-s}, and are given in formulas 4.331.1, 4.335.1, and 4.335.3 of I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products,* corrected and enlarged edition (Academic, New York, 1980).

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