Resonant Activation over a Fluctuating Barrier

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We consider the problem of thermally activated potential barrier crossing in the presence of fluctuations of the barrier itself. For a piecewise linear barrier switching between two values as a Markov process, exact and Monte Carlo results reveal a novel resonantlike phenomenon as a function of the barrier fluctuation rate. For very slow variations the average crossing time is the average of the times required to diffuse over each of the barriers separately; for very fast variations the mean crossing time is that required to cross the average barrier. At intermediate rates the crossing is strongly correlated with the potential variation and the escape rate exhibits a local maximum at a "resonant" fluctuation rate.

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Ever since the pioneering work of Kramers [1], the problem of diffusion over potential barriers has held a central role in statistical physics, providing a microscopic mechanism for the Arrhenius temperature dependence of crossing rates [2]. Several variations of the basic model have been introduced recently for the study of more complex nonequilibrium systems, including diffusion over a barrier in the presence of a harmonic force [3] and diffusion over a fluctuating barrier [4–7]. The hallmark of the former situation is the phenomenon of "stochastic resonance" where the signal-to-noise ratio of the system's response to the applied harmonic force displays a local maximum as a function of the diffusion coefficient (or the temperature). In this paper we report a novel resonantlike behavior in the latter case of diffusion over a fluctuating barrier. For very slow variations the average crossing time is the average of the times required to diffuse over each of the barriers, while for very fast variations the average crossing time is that required to cross the average barrier. These limiting cases are in accord with intuitive expectations. At intermediate rates, however, the crossing is strongly correlated with the potential fluctuations and the escape rate exhibits a maximum at a resonant fluctuation rate.

We study the problem of overdamped thermal activation in the presence of barrier fluctuations for a piecewise linear potential barrier switching between two values as a Markov process. We present both exact and Monte Carlo results for the mean first-passage time (MFPT) of the diffusion process which display a local minimum, signaling resonant activated barrier crossing, as a function of the barrier fluctuation rate. Exact results for diffusion over a (fixed) piecewise linear potential barrier have recently been obtained [8], as have exact results for the non-Markovian MFPT problem for processes driven by the dichotomous Markov process [9], and by a dichotomous Markov process coupled to a diffusion process [10]. Earlier studies of activation over fluctuating barriers were restricted to limiting cases, i.e., slow [4] or fast [4,5] barrier fluctuations, or small fluctuations (low temperature) [6]. Not unexpectedly, the resonant activation phenomenon observed in the new exact results reported here is absent in those approximate treatments.

The rest of this paper is organized as follows. We next describe our model of activation over a fluctuating barrier and indicate the modes of analysis that are brought to bear in its study. Exact and Monte Carlo results are then presented to both illustrate the resonant activation and provide an understanding of the mechanism responsible for this behavior. We conclude with a brief discussion of our results, pointing out some open questions.

The (overdamped) state variable $X(t)$ moves in the fluctuating potential $V(x,t)$ under the influence of a heat bath at temperature T, so the state variable satisfies the stochastic differential equation

$$\frac{dX}{dt} = -V'(X,t) + \sqrt{2T}\,\xi(t)\,, \tag{1}$$

where $\xi(t)$ appearing in the Langevin force term is a Gaussian white noise process with

$$\langle \xi(t)\xi(s)\rangle = \delta(t-s)\,. \tag{2}$$

In the above, V' denotes the derivative of the potential V with respect to x, the particle mass and Boltzmann's constant have been set to 1, and time is measured in terms of the friction coefficient (also set to 1) [11]. The setup for the model is shown in Fig. 1. We take the potential to be fluctuating randomly between two configurations, $V_+(x)$ and $V_-(x)$, as a Markov process—the potential remains

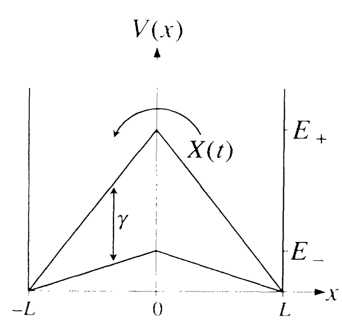

FIG. 1. Setup for the problem. The center height of the triangular potential barrier fluctuates between E_+ and E_- at rate γ.

in one state for an exponentially distributed random time before switching to the other. That is, the probabilities $P_\pm(t)$ that $V(x,t)=V_\pm(x)$ satisfy the master equation

$$\frac{d}{dt}\begin{pmatrix}P_+\\P_-\end{pmatrix}=\begin{pmatrix}-\gamma & \gamma\\ \gamma & -\gamma\end{pmatrix}\begin{pmatrix}P_+\\P_-\end{pmatrix}. \tag{3}$$

The parameter γ is the flipping rate of the barrier, and its inverse is the average time that the barrier stays in one configuration before switching to another. In the first-passage problem that we consider the state variable starts off at position L (the bottom of a well of the potentials) with the barrier in the $\pm$ state with probability $\frac{1}{2}$, and is absorbed at position 0 (the top of the potentials).

The problem as outlined above may be studied via Monte Carlo simulation. Direct numerical solution of the stochastic differential equation is carried out using well-known methods [12], and first-passage times of the process $X(t)$ from L to 0 are collected for statistical analysis, for example, for measurement of the mean first-passage time (MFPT). We note that potential shapes more general than piecewise linear potentials can also be simulated, but we restrict our attention to these simple shapes in order to complement a purely numerical study with exact theoretical results as described next.

The composite system, comprising both the state variable and fluctuating potential barrier, is described analytically by the joint probability density $\rho_\pm(x,t)$ that $X(t)=x$ and that the potential is in the $\pm$ configuration. This joint probability satisfies the coupled Fokker-Planck equations

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho_+\\\rho_-\end{pmatrix}=\begin{pmatrix}-\gamma+\frac{\partial}{\partial x}\left\{V_+'(x)+T\frac{\partial}{\partial x}\right\} & \gamma\\ \gamma & -\gamma+\frac{\partial}{\partial x}\left\{V_-'(x)+T\frac{\partial}{\partial x}\right\}\end{pmatrix}\begin{pmatrix}\rho_+\\\rho_-\end{pmatrix}. \tag{4}$$

The appropriate initial and boundary conditions for Eq. (4) are

$$\rho_\pm(x,0)=\tfrac{1}{2}\delta(x-L) \tag{5}$$

and

$$\rho_\pm(x,t)|_{x=0}=0. \tag{6}$$

For $t>0$ we impose reflecting boundary conditions (vanishing probability current) at the walls of the potentials:

$$-\left\{V_\pm'(x)+T\frac{\partial}{\partial x}\right\}\rho_\pm(x,t)\Bigg|_{x=L}=0. \tag{7}$$

The probability that the first-passage time τ from L to 0 is greater than t is obtained from the solution to Eqs. (4)-(7) according to

$$F(t):=\mathrm{Prob}\{\tau>t\}=\int_0^L[\rho_+(x,t)+\rho_-(x,t)]dx. \tag{8}$$

All of the statistics of τ can be computed from $F(t)$, for example, the MFPT is

$$\langle\tau\rangle=\int_0^\infty F(t)dt. \tag{9}$$

The general solution to Eqs. (4)-(7) for arbitrary potentials $V_\pm$ is not known, which is the reason for our concentrating on the simple piecewise linear profiles as shown in Fig. 1. Then the equations for $\rho_\pm$ are linear constant coefficient partial differential equations which may be solved by standard methods. Even with this simplification, the exact expression for the MFPT is generally quite complicated However, in the case where the midpoint of the barrier fluctuates between $\pm E$ (that is, where $E_+=-E_-=E$) it is simple enough to summarize analytically. Then the MFPT from L to 0 is, explicitly,

$$\langle\tau\rangle T/L^2=A_-\left\{-\frac{E}{Tk}(1-e^k)+\frac{\gamma L^2k}{E}-\frac{E}{T}\right\}+A_+\left\{\frac{E}{Tk}(1-e^{-k})-\frac{\gamma L^2k}{E}-\frac{E}{T}\right\}, \tag{10a}$$

where

$$A_\pm=-\frac{(2\gamma L^2/T)(\pm e^{\pm k}-k)\pm E^2/T^2}{2(Ek/T)(1+2\gamma L^2T/E^2)[(2\gamma L^2/T)\cosh k+E^2/T^2]}, \tag{10b}$$

and

$$k=\left(\frac{E^2}{T^2}+\frac{2\gamma L^2}{T}\right)^{1/2}. \tag{10c}$$

A plot of the dimensionless MFPT $\langle\tau\rangle T/L^2$ versus the dimensionless barrier fluctuation rate $\gamma L^2/T$ is given in Fig. 2 for the parameter values $E=8T$, displaying the resonant activation phenomenon. For very slow barrier fluctuation rates—significantly slower than the time required to cross the highest barrier—the MFPT approaches the average of the MFPTs for the alternative barrier configurations:

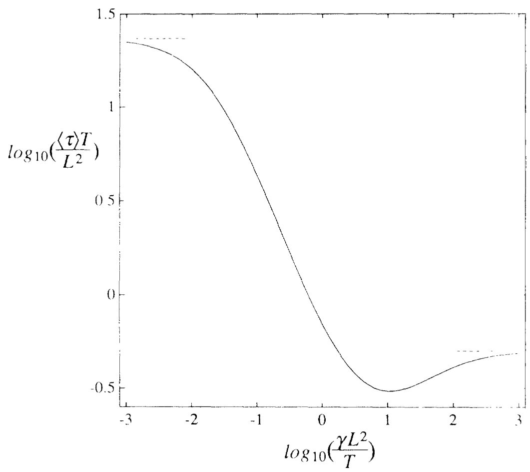

FIG. 2. MFPT vs barrier fluctuation rate for the parameter values $E_\pm = \pm 8T$. Dashed lines indicate limiting values of the MFPT for slow or fast variations.

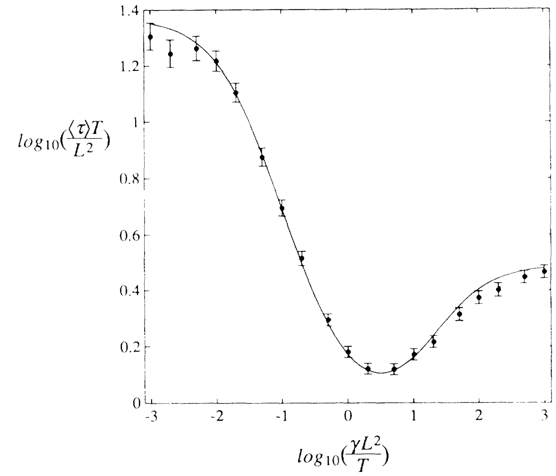

FIG. 3. MFPT vs barrier fluctuation rate for the parameter values $E_+ = 8T$ and $E_- = 0$. Solid line: theoretical curve. Discrete data: Monte Carlo simulations (2σ error bars).

$$\langle\tau\rangle T/L^2 \xrightarrow[\gamma L^2/T\to 0]{} \frac{1}{2}\frac{T^2}{E^2}\left[e^{+E/T}-1-\frac{E}{T}\right]+\frac{1}{2}\frac{T^2}{E^2}\left[e^{-E/T}-1+\frac{E}{T}\right]. \tag{11}$$

On the other hand, for barrier fluctuations fast compared to the typical crossing time, the MFPT approaches that required to cross the average barrier, $\langle E\rangle = E_+/2 + E_-/2$:

$$\langle\tau\rangle T/L^2 \xrightarrow[\gamma L^2/T\to \infty]{} \frac{T^2}{\langle E\rangle^2}\left[e^{+\langle E\rangle/T}-1-\frac{\langle E\rangle}{T}\right]=\frac{1}{2}. \tag{12}$$

At intermediate times, however, the MFPT is less than either of these limits. The MFPT has a local minimum for a value of the barrier fluctuation rate on the order of the inverse of the time required to cross in the "down" configuration. This suggests that while the crossing event is independent of the barrier configuration in either of the two limiting cases ($\gamma \to 0$ or $\gamma \to \infty$), it is strongly correlated with the potential fluctuations at intermediate times where the crossing takes place preferentially when the barrier is in its lower configuration.

Another example is plotted in Fig. 3. Here the top of the barrier fluctuates between $E_+ = 8T$ and $E_- = 0$ The theoretical curve (solid line) is the exact solution, although a symbolic manipulation program was required to perform all the algebra. The discrete data are from Monte Carlo simulations [13]. The results of the symbolic manipulation and the direct simulation are in excellent agreement, serving as checks for each other's validity and precision. The resonant activation behavior is again apparent in Fig. 3.

The Monte Carlo simulations yield more information about the activation process. In order to check the idea that the resonance occurs when the crossing takes place with the barrier most likely in the down position, we kept track of the position of the barrier at the instant that the state variable reached $x=0$. In Fig. 4 we plot the probability that the barrier is in the down configuration at the instant of crossing versus the dimensionless barrier fluctuation rate for the same parameter values as in Fig. 3. In the limits of very fast or very slow variations of the barrier's position, it is equally likely to be up or down at the moment of crossing. In the neighborhood of the resonant activation, when the time scale of the flipping is of the order of the MFPT across the lower barrier, the crossing occurs almost exclusively when the barrier is in the lower state.

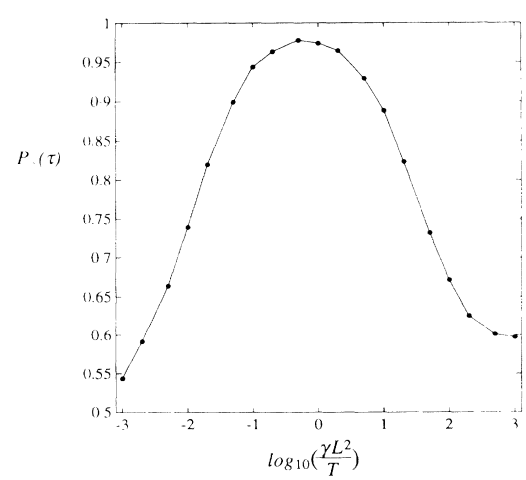

FIG. 4. Probability that the barrier is in the down configuration at the instant of crossing vs barrier fluctuation rate, from Monte Carlo simulations with the same parameter values as in Fig. 3. Solid line is a guide to the eye.

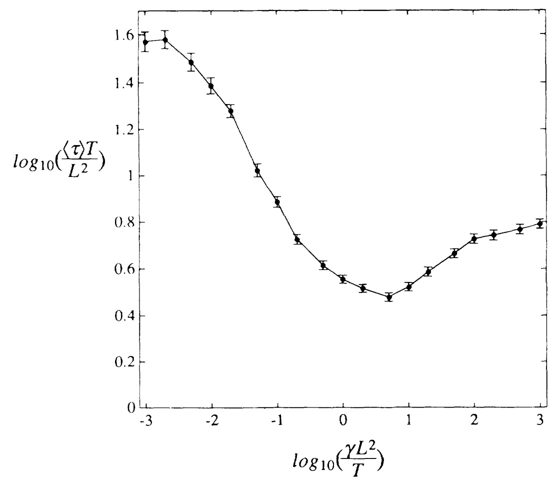

FIG. 5. Monte Carlo data (2σ error bars) for the MFPT all the way across the barrier vs the barrier fluctuation rate for the parameters $E_+ = 8T$ and $E_- = 0$. Solid line is a guide to the eye.

In Fig. 5 we plot Monte Carlo data for the MFPT all the way across the barrier, i.e., from $x = L$ to $x = -L$, versus the barrier fluctuation rate for the parameter values $E_+ = 8T$ and $E_- = 0$. This confirms that the resonant activation phenomenon is not an artifact of our computing the time required to go only to the middle of the interval [14].

There are a number of further studies suggested by the results presented here. The phenomenon we have observed for these piecewise linear barriers reveals the physical mechanism of resonant activation over a fluctuating barrier in a simple model system with the most fundamental type of fluctuation. This raises the question of both quantitative and qualitative effects of other potential shapes and/or fluctuation statistics. For example, is the resonance narrowed in other models? Additionally, the probability distribution of the first-passage time across the barrier is of interest. Is there a qualitative difference in the first-passage time distribution near, as opposed to far from, the resonant activation? The motivation for considering activation over fluctuating potential barriers in Ref. [4] was to study models of relaxation in complex many-body systems. The idea introduced there is that the barrier to relaxation in a subsystem may be built up from like subsystems with similar fluctuation dynamics. To fully investigate these kinds of models one needs at least to include a relationship between the barrier's fluctuation time scale and the crossing time scale (in, say, a self-consistent manner). Further investigation of these problems is left to a future study.

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