Diffusive hysteresis at high and low driving frequencies

James Christopher Phillips and Klaus Schulten
Department of Physics and Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 5 May 1995)

The hysteresis loop area of a diffusive system in a sinusoidally driven potential is studied. Asymptotic expansions of the hysteresis loop area are constructed in the high and low driving frequency limits. Kramers' approximation is used to construct a simplified expansion in the limit of both low driving frequency and low temperature. The driving force is never assumed to be small.

PACS number(s): 05.40.+j, 02.50.−r

I. INTRODUCTION

Hysteresis is the nonlinear and time-delayed response of a system to the cyclical variation of a control parameter, a familiar example being changes in magnetization in response to a magnetic field. Often, hysteresis depends on the frequency with which the control parameter is varied. This may be modeled as the overdamped dynamics of a particle in a bistable potential. When random noise is added to such a system we obtain a Langevin equation, for which a diffusion description via the Smoluchowski equation is appropriate.

Periodically driven stochastic systems have been the subject of recent study, particularly concerning the phenomenon of stochastic resonance. For an overview, the reader is directed to a review by Jung [1]. Theoretical efforts have been made towards understanding these systems via assumptions of large [2] and small [2–5] driving frequencies, two-state approximations [6], linear response theory [6–8], and perturbation theory [9]. Unfortunately, most of these efforts have been limited to small driving amplitudes, the domain of interest in stochastic resonance. Except for numerical studies [10], hysteresis in these systems has received little attention. Future areas to which the theory of driven stochastic systems may be applied include atomic force microscopy [11] and the dipole response of proteins to external electric fields [12].

In this paper we study hysteresis in a one-dimensional diffusive system which is subjected to sinusoidal forcing of arbitrary amplitude. In Sec. I A we describe the system to be studied and define the hysteresis loop area. In Sec. I B we describe briefly the numerical methods used to verify our results. In Secs. II and III we derive asymptotic expansions for the area of the hysteresis loop in the high and low frequency limits which are applicable to any potential of the form $V(X)+\sin(\Omega t)\,W(X)$. The high frequency expansion is found to be simple and independent of temperature, while the low frequency expansion requires multiple quadratures. The expansions are verified by numerical integration of the Smoluchowski equation. In Sec. IV we employ Kramers' approximation to propose a simplified model for the driven double-well Landau potential at low temperatures in the low frequency limit and extract an expansion for the hysteresis loop area from this model. The result does not depend on the driving amplitude, aside from an assumption that it is *not* small. The Kramers expansion is verified by comparison with the general low frequency expansion of Sec. III.

A. Statement of problem

We wish to study hysteresis in a general sense for a sinusoidally perturbed stochastic system. We make no assumptions about the strength of the perturbation. We assume that the high friction limit is applicable, i.e., the system is described by the one-dimensional Smoluchowski equation.

We consider diffusion in a potential $U(X,t) = V(X) + \sin(\Omega t)\,W(X)$, where $U(X,t) \to +\infty$ as $X \to \pm\infty$ for all times t. The evolution of a probability distribution $P(X,t)$ is governed by the Smoluchowski equation [13,14]

$$\partial_t P(X,t) = \partial_X D\left[\partial_X + \frac{1}{k_B T}[V_X(X) + \sin(\Omega t)\,W_X(X)]\right]P(X,t), \qquad (1)$$

where the subscripts on V and W denote differentiation with respect to X. Note that the diffusion constant D may be expressed in a temperature-dependent manner as $k_B T/\gamma$, where γ is the friction coefficient in the Langevin equation $m\ddot{X} = -\partial_X U(X,t) - \gamma\dot{X} + \sigma\xi(t)$. At long times the distribution becomes time periodic with frequency Ω. This *asymptotic* distribution $P_{\rm as}(X,t)$ may be expanded in a Fourier series as $A_0(X) + A_1(X)\cos(\Omega t) + B_1(X)\sin(\Omega t) + \cdots$. In this paper we are only concerned with asymptotic distributions and, therefore, drop the subscript "as" from here forward.

We now make substitutions to reduce the number of parameters in the problem. Introducing the dimensionless quantities $x \equiv X/X_0$, $p \equiv X_0 P$, $u \equiv U/U_0$, $v \equiv V/U_0$, $w \equiv W/U_0$, and $\theta \equiv \Omega t$ transforms (1) into

$$\left(\frac{\Omega}{X_0}\right)\partial_\theta p(x,\theta) = \left(\frac{k_B T}{X_0^3\gamma}\right)\partial_x\left[\partial_x + \frac{U_0}{k_B T}[v_x(x) + \sin\theta\, w_x(x)]\right]\left(\frac{1}{X_0}\right)p(x,\theta). \quad (2)$$

Defining the parameters $\tau \equiv 1/\beta \equiv k_B T/U_0$ and $\omega \equiv \Omega X_0^2\gamma/U_0$ produces the final form

$$\omega\partial_\theta p(x,\theta) = \partial_x\left[\tau\partial_x + v_x(x) + \sin\theta\, w_x(x)\right]p(x,\theta). \quad (3)$$

Except for the forms of the potentials v and w, there are only two parameters of consequence: ω, which characterizes the driving frequency relative to the relaxation time of the system *excluding barrier-hopping processes*; and τ, which characterizes the temperature of the system relative to the scale of the potential U, and therefore *does* describe barrier-hopping processes. We assume that v, w, and p are of order unity, allowing us to consider independently the magnitudes of the parameters ω and τ.

The hysteresis loop area $\mathcal{H}$ of such a system can be defined as the area enclosed by a plot of the mean $\mu_p(\theta)$ of the distribution $p(x,\theta)$ versus $\sin\theta$. Assuming that $[\sin\theta, \mu_p(\theta)]$ forms a loop in the positive sense we have

$$\mathcal{H} \equiv -\oint \mu_p(\theta)\, d\sin\theta \quad (4a)$$

$$= -\pi\int_{-\infty}^{\infty} x\, a_1(x)\, dx, \quad (4b)$$

where $a_1(x)$ is the $\cos\theta$ Fourier component of $p(x,\theta)$.

B. Numerical examples

To verify the asymptotic expansions developed in Secs. II and III we numerically integrate (3) for a prototypical bistable potential $v(x) = x^4/4 - x^2/2$. This symmetric potential has wells at $x = \pm 1$ and a barrier of height 1/4 at $x = 0$. For the sinusoidally driven perturbing potential we select $w(x) = -\alpha\, x$, a choice which ensures that $\mathcal{H}$ is positive. For our numerical integrations we take $\alpha = 1/2$, which is sufficient to overcome the central barrier and "dump" the distribution between the wells.

The calculations employ standard fully implicit methods for the time propagation of diffusion equations, as outlined in [15]. The asymptotic distribution is found by integrating forward in time from an initial Boltzman distribution at $\theta = 0$ until $p(\theta)$ and $p(\theta + 2\pi)$ do not differ significantly. This distribution is then renormalized and integration continues for one additional cycle to collect data. The final distribution then serves as the initial distribution for a system with slightly altered parameters. The method is simple and effective, but suffers at extremely small ω.

II. HIGH FREQUENCY LIMIT

In this section we construct an asymptotic expansion [16] for the hysteresis loop area in the high frequency limit: we derive an expression for $\mathcal{H}$ which is correct to first order in ω^{-1}. The result is simple and, in the case of a constant perturbing force, independent of temperature. Comparison with values of the hysteresis loop area calculated via numerical integration of the Smoluchowski equation verifies the formula.

Assuming $\omega \gg 1$, we expand $p(x,\theta)$ as a power series $p(x,\theta) = p_0(x,\theta) + \omega^{-1}p_1(x,\theta) + O(\omega^{-2})$. This is then substituted into (3) to yield

$$\partial_\theta\left[\omega p_0(x,\theta) + p_1(x,\theta) + O(\omega^{-1})\right] = \partial_x\left[\tau\partial_x + v_x(x) + \sin\theta\, w_x(x)\right]\left[p_0(x,\theta) + \omega^{-1}p_1(x,\theta) + O(\omega^{-2})\right]. \quad (5)$$

Beginning with the highest order terms, we now match powers of ω to produce a series of simpler equations for the p_n.

There is only one term of order ω, therefore $\partial_\theta p_0(x,\theta) = 0$. At large driving frequencies the response time of the system is much slower than the oscillations in $\sin\theta$. This allows us to ignore $w(x)$ in the limit $\omega \to \infty$. Thus $p_0(x,\theta) = Ne^{-\beta v(x)}$, where $N^{-1} = \int_{-\infty}^{\infty} e^{-\beta v(x)}\, dx$. Matching terms of order ω^0 produces the equation $\partial_\theta p_1(x,\theta) = \partial_x\left[\tau\partial_x + v_x(x) + \sin\theta\, w_x(x)\right]p_0(x,\theta)$. By substituting the above expression for $p_0(x,\theta)$ we reduce this to $\partial_\theta p_1(x,\theta) = N\partial_x \sin\theta\, w_x(x)e^{-\beta v(x)}$. Integration with respect to θ then yields $p_1(x,\theta) = -N\partial_x w_x(x)e^{-\beta v(x)}\cos\theta + f(x)$ where $f(x)$ is an arbitrary function, conditioned only by $\int_{-\infty}^{\infty} f(x)\, dx = 0$. Therefore, our asymptotic expansion for the distribution is

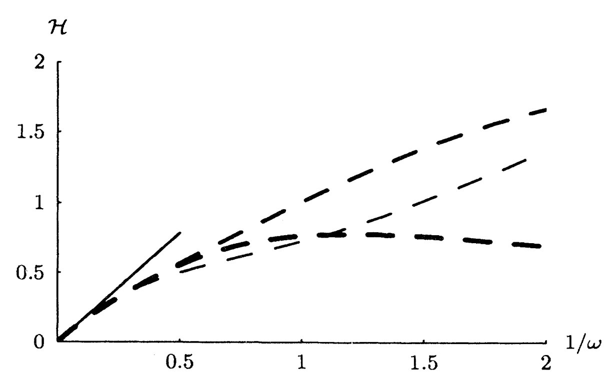

FIG. 1. Hysteresis loop area in the high frequency limit: comparison of asymptotic expansion (7) (continuous line) with results of numerical integration of the Smoluchowski equation (3) for $v(x) = x^4/4 - x^2/2$ and $w(x) = -\alpha\, x$ with $\alpha = 1/2$ (broken lines). Plots represent $\tau = 1/16$ (thin line), 1/4 (medium line), and 1 (thick line).

$$p(x,\theta) = Ne^{-\beta v(x)} + \omega^{-1}[-N\partial_x w_x(x) e^{-\beta v(x)}\cos\theta + f(x)] + O(\omega^{-2}). \quad (6)$$

To calculate the hysteresis loop area, we use (4b). By inspection of (6) we obtain $a_1(x) = -\omega^{-1}N\partial_x w_x(x)e^{-\beta v(x)} + O(\omega^{-2})$. Integration by parts yields $\mathcal{H} = -\pi\omega^{-1}N\int_{-\infty}^{\infty} w_x(x)e^{-\beta v(x)}\,dx + O(\omega^{-2})$, which can be simplified as

$$\mathcal{H} = -\pi\,\omega^{-1}\left\langle w_x(x)\right\rangle_{p_0} + O(\omega^{-2}). \quad (7)$$

When $w(x) = -\alpha x$, this simplifies further to $\mathcal{H} = \pi\,\alpha\,\omega^{-1} + O(\omega^{-2})$ which is independent of temperature. This result has been verified by numerical integration of (3) via the method of Sec. I B, as shown in Fig. 1. A similar result has been found for magnetic systems [17,18].

III. LOW FREQUENCY LIMIT

In this section we construct an asymptotic expansion [16] for the hysteresis loop area in the low frequency limit: we derive an expression for $\mathcal{H}$ which is correct to first order in ω. The result is complicated, requiring multiple quadratures for its evaluation. Fortunately, the calculation can be performed numerically and in Sec. IV we obtain a simple expression for the low temperature limit of our prototypical system. Comparison with values of the hysteresis loop area calculated via numerical integration of the Smoluchowski equation verifies the formula.

Assuming $\omega \ll 1$, we expand $p(x,\theta)$ as a power series $p(x,\theta) = p_0(x,\theta) + \omega p_1(x,\theta) + O(\omega^2)$. This is then substituted into (3) to yield

$$\partial_\theta\left[\omega p_0(x,\theta) + \omega^2 p_1(x,\theta) + O(\omega^3)\right] = \partial_x\left[\tau\partial_x + v_x(x) + \sin\theta\, w_x(x)\right]\left[p_0(x,\theta) + \omega p_1(x,\theta) + O(\omega^2)\right]. \quad (8)$$

Beginning with the lowest order terms, we now match powers of ω to produce a series of simpler equations for the p_n.

Since there is only one term of order ω^0, we have for the first equation $\partial_x[\tau\partial_x + v_x(x) + \sin\theta\, w_x(x)]p_0(x,\theta) = 0$. This has the obvious solution $p_0(x,\theta) = N(\theta)e^{-\beta[v(x)+\sin\theta\, w(x)]}$, where $N^{-1} = \int_{-\infty}^{\infty} e^{-\beta[v(x)+\sin\theta\, w(x)]}\,dx$. Note that here, in contrast to Sec. II, N is θ dependent. Matching terms of order ω yields the equation $\partial_\theta p_0(x,\theta) = \partial_x\left[\tau\partial_x + v_x(x) + \sin\theta\, w_x(x)\right]p_1(x,\theta)$. An inhomogeneous equation, this has the solution $p_1(x,\theta) = M(\theta)p_0(x,\theta) + f(x,\theta)$, where $f(x,\theta)$ is a specific solution yet to be determined. The normalization condition $\int_{-\infty}^{\infty} p_1(x,\theta)\,dx = 0$ allows us to express $M(\theta) = -\int_{-\infty}^{\infty} f(x,\theta)\,dx$. Therefore, we need only determine $f(x,\theta)$.

By rewriting the order-ω equation as $\partial_\theta p_0(x,\theta) = \tau\partial_x e^{-\beta u(x,\theta)}\partial_x e^{\beta u(x,\theta)} f(x,\theta)$ we can find f through integration. First we write $\beta\int_a^x \partial_\theta p_0(x',\theta)\,dx' = e^{-\beta u(x,\theta)}\partial_x e^{\beta u(x,\theta)} f(x,\theta)$. We select the lower bound of integration $a = -\infty$ because this choice ensures that the expression is zero at $x = \pm\infty$. Repeating the integration, we obtain $\beta\int_b^x e^{\beta u(x',\theta)}\int_{-\infty}^{x'}\partial_\theta p_0(x'',\theta)\,dx''dx' = e^{\beta u(x,\theta)} f(x,\theta)$. Since the value of the integration limit b can be absorbed into $M(\theta)$, we pick $b = 0$ for convenience. Thus, our final expression for the specific solution is

$$f(x,\theta) = \beta e^{-\beta u(x,\theta)}\int_0^x e^{\beta u(x',\theta)} \times\left(\int_{-\infty}^{x'}\partial_\theta N(\theta)e^{-\beta u(x'',\theta)}\,dx''\right)dx' \quad (9)$$

and our expansion of the distribution is

$$p(x,\theta) = N(\theta)e^{-\beta u(x,\theta)} + \omega\left[f(x,\theta) - \left(\int_{-\infty}^{\infty} f(x',\theta)\,dx'\right)N(\theta)e^{-\beta u(x,\theta)}\right] + O(\omega^2). \quad (10)$$

$\mathcal{H}$ may then be calculated by the straightforward application of (4) to (10). The calculations themselves are a series of quadratures and may be performed numerically. This has been done and in Fig. 2 the results are compared to those obtained by numerical integration of (3) via the method of Sec. I B. Note that the expansion grows quite steep with increasing β, as is further commented on in Sec. IV.

IV. LOW TEMPERATURE, LOW FREQUENCY LIMIT

In this section we employ Kramers' approximation [19] for the barrier-hopping rate to construct an approximation for the hysteresis loop area of our prototypical system in the low temperature, low frequency limit. Similar methods have been used to address stochastic resonance

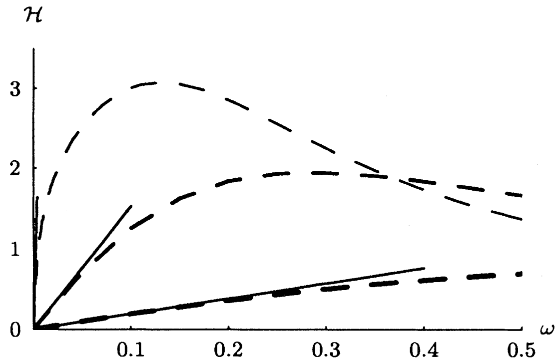

FIG. 2. Hysteresis loop area in the low frequency limit: comparison of $\mathcal{H}$ calculated from asymptotic expansion (10) (continuous lines) with results of numerical integration of the Smoluchowski equation (3) for $v(x) = x^4/4 - x^2/2$ and $w(x) = -\alpha x$ with $\alpha = 1/2$ (broken lines). Plots represent $\tau = 1/16$ (thin line), 1/4 (medium line), and 1 (thick line).

[4,5]. Kramers' approximation is only valid with large barrier heights, but we can employ it successfully with large perturbing forces because we are in the adiabatic limit. We make the additional approximations that the positions and curvatures of the extrema do not change as the system is perturbed and that the mean of the distribution in each well remains at the corresponding minimum of the unperturbed system. The result is simple and matches the more complicated result of Sec. III surprisingly well.

Kramers' approximation for the transition rate over a high barrier is $k_{\text{escape}} = \omega_{\text{well}}\omega_{\text{barrier}}\,(2\pi\gamma)^{-1}\,e^{-\beta u_{\text{barrier}}}$, where u_{barrier} is the barrier height and ω^2_{well} and $-\omega^2_{\text{barrier}}$ are the curvatures of u at the bottoms of the wells and at the top of the barrier, respectively. In our prototypical bistable potential $u(x,\theta) = x^4/4 - x^2/2 - \alpha x \sin\theta$ we approximate the full diffusion problem by the fractions of particles in the left and right wells, N_A and N_B, and the Kramers escape rates from them, k_A and k_B. These are related by

$$\dot{N}_A = -k_A N_A + k_B N_B, \tag{11a}$$

$$\dot{N}_B = -k_B N_B + k_A N_A. \tag{11b}$$

Kramers' approximation is only valid for $u_{\text{barrier}} \gg \tau$. However, if our system is in the adiabatic limit and the temperature of the system is low then almost all of the flux occurs within a short time of when the side with the lower well changes. Therefore, Kramers' approximation need only be valid near this time of high flux for the model as a whole to be correct. Hence, we are allowed to make the rough approximation that the wells remain at ± 1 and the barrier at 0 for all θ, providing approximate escape rates of $k_A = \left(\sqrt{2}\pi\gamma\right)^{-1} e^{-\beta(1/4-\alpha\sin\theta)}$ and $k_B = \left(\sqrt{2}\pi\gamma\right)^{-1} e^{-\beta(1/4+\alpha\sin\theta)}$. We also approximate the means of the distributions in the wells by ± 1, resulting in an overall mean $\mu_p = N_B - N_A$. This approximation is inaccurate at large driving amplitudes, but the errors are mainly in phase with the driving force and, therefore, do not contribute to the hyteresis. We use our definition of μ_p and the normalization condition $N_A + N_B = 1$ to rewrite (11), after some manipulation, as

$$\omega e^{\beta/4}\,\partial_\theta \mu_p(\theta) = \frac{\sqrt{2}}{\pi}\,[\sinh(\alpha\beta\sin\theta) - \mu_p(\theta)\cosh(\alpha\beta\sin\theta)]. \tag{12}$$

Since we are in the adiabatic limit, we assume $\omega \ll e^{-\beta/4}$ and construct an asymptotic expansion in the small parameter $\varepsilon = \omega e^{\beta/4}$.

Expanding $\mu_p(\theta) = \mu_0(\theta) + \varepsilon\mu_1(\theta) + O(\varepsilon^2)$ and substituting into (12) yields the order ε^0 equation $0 = (\sqrt{2}/\pi)\,[\sinh(\alpha\beta\sin\theta) - \mu_0(\theta)\cosh(\alpha\beta\sin\theta)]$. Thus, $\mu_0(\theta) = \tanh(\alpha\beta\sin\theta)$. Resubstituting and matching terms of order ε produces $\alpha\beta\cos\theta\,\mathrm{sech}^2(\alpha\beta\sin\theta) = -(\sqrt{2}/\pi)\,\mu_1(\theta)\cosh(\alpha\beta\sin\theta)$, so $\mu_1(\theta) = -(\alpha\beta\pi/\sqrt{2})\cos\theta\,\mathrm{sech}^3(\alpha\beta\sin\theta)$. Our full expansion for $\mu_p(\theta)$ is then

$$\mu_p(\theta) = \tanh(\alpha\beta\sin\theta) - \varepsilon(\alpha\beta\pi/\sqrt{2})\cos\theta\,\mathrm{sech}^3(\alpha\beta\sin\theta) + O(\varepsilon^2). \tag{13}$$

Applying (4) to (13) gives

$$\mathcal{H} \sim e^{\beta/4}\,(\alpha\beta\omega\pi/\sqrt{2}) \int_0^{2\pi} \cos^2\theta\,\mathrm{sech}^3(\alpha\beta\sin\theta)d\theta\ ,$$

which cannot be expressed in closed form. However, since we have assumed $\beta \gg 1$, we can make the additional assumption that $\alpha\beta \gg 1$ and expand around the (very

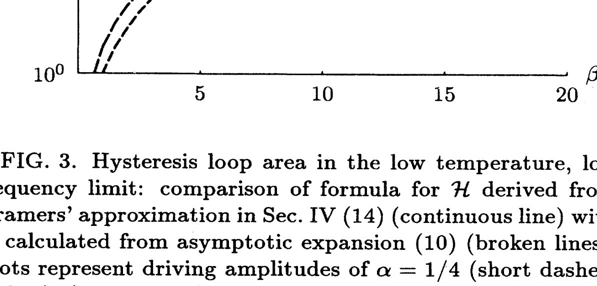

FIG. 3. Hysteresis loop area in the low temperature, low frequency limit: comparison of formula for $\mathcal{H}$ derived from Kramers' approximation in Sec. IV (14) (continuous line) with $\mathcal{H}$ calculated from asymptotic expansion (10) (broken lines). Plots represent driving amplitudes of $\alpha = 1/4$ (short dashes) and 1/2 (long dashes).

sharp) peaks of $\mathrm{sech}^3(\alpha\beta\sin\theta)$ at $\theta = 0, \pi$. This leads to $\mathcal{H} \sim \omega\, e^{\beta/4}\, \pi\sqrt{2} \int_{-\infty}^{\infty} \mathrm{sech}^3(x) dx$, which can be expressed in closed form. Hence, our approximation assumes the final form

$$\mathcal{H} \sim \frac{\omega\, e^{\beta/4}\, \pi^2}{\sqrt{2}} \quad \left(\beta \gg 1,\ \alpha\beta \gg 1,\ \omega \ll e^{-\beta/4}\right). \quad (14)$$

To verify (14), we compare it to the result of Sec. III. As shown in Fig. 3, the two methods agree in the large β regime. This agreement is particularly surprising when one considers the number of approximations which entered into our calculation. Another pleasant surprise is that our approximation is α independent aside from the conservative assumption that $\alpha\beta \gg 1$. This restriction is not too disappointing, however, because if α is small the problem may be addressed via linear response theory. The large growth rate of the expansion with increasing β, when combined with the fact that the hysteresis loop area is bounded, can provide an estimate for the range of applicability of the low frequency expansion.

ACKNOWLEDGMENTS

We thank Peter Jung for his helpful comments. J.C.P. thanks the Fannie and John Hertz Foundation and the University of Illinois for support. This work was supported by grants from the National Institutes of Health (PHS 5 P41 RR05969-04) and the Roy J. Carver Charitable Trust.

[1] P. Jung, Phys. Rep. **234**, 175 (1993).
[2] P. Jung, Z. Phys. B. **76**, 521 (1989).
[3] L. Gammaitoni, E. Menichella-Saetta, S. Santucci, and F. M. and C. Presilla, Phys. Rev. A **40**, 2105 (1989).
[4] B. McNamara and K. Wiesenfeld, Phys. Rev. A **39**, 4854 (1989).
[5] G. Hu, H. Haken, and C. Z. Ning, Phys. Rev. E **47**, 2321 (1993).
[6] P. Jung and P. Hanggi, Z. Phys. B **90**, 255 (1993).
[7] G. Hu, H. Haken, and C. Z. Ning, Phys. Lett. A **172**, 21 (1992).
[8] M. I. Dykman *et al.*, Phys. Lett. A **180**, 332 (1993).
[9] C. Presilla, F. Marchesoni, and L. Gammaitoni, Phys. Rev. A **40**, 2105 (1989).
[10] M. C. Mahato and S. R. Shenoy, Phys. Rev. E **50**, 2503 (1994).
[11] J. Phillips and K. Schulten, in *NATO Advanced Research Workshop on Atomic Force Microscopy, NATO Advanced Study Institute, Series B: Physics*, edited by J. P. Rabe and H. Gaub (Kluwer, in press).
[12] D. Xu and K. Schulten (unpublished).
[13] H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1984).
[14] C. W. Gardiner, *Handbook of Stochastic Methods* (Springer, Berlin, 1983).
[15] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd ed. (Cambridge, Cambridge, 1992).
[16] E. J. Hinch, *Perturbation Methods* (Cambridge, Cambridge, 1991).
[17] D. Dhar and P. B. Thomas, J. Phys. A **25**, 4967 (1992).
[18] M. Rao, H. R. Krishnamurthy, and R. Pandit, Phys. Rev. B **42**, 856 (1990).
[19] H. A. Kramers, Physica (The Hague) **7**, 284 (1940).