Semianalytic solution of the Kramers exit problem for a small ferromagnetic particle

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The distribution $Q(t)$ of magnetization reversal times in a small uniaxial particle is computed here directly from Brown's Fokker-Planck equation. Constant applied field and axial symmetry are assumed. The Laplace transform of $Q(t)$ has the form $\hat{Q}(z)=F_1(z)/F_2(z)$ where the regular functions $F_i(z)$ are defined by a solution of a Volterra integral equation. A separate integral equation is derived for the function $dF_2(z)/dz$, and the poles and residues of $\hat{Q}(z)$ may then be found numerically with arbitary precision. [S1063-651X(99)07006-3]

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I. INTRODUCTION

The Kramers exit problem [1] for a small ferromagnetic particle was formulated by Brown [2] who wrote down the relevant Fokker-Planck equation and calculated the thermal relaxation rate κ for a uniaxial particle in external magnetic field applied parallel to its easy axis. The thermal relaxation rate is the single parameter of the Markovian decay law $W(t)=e^{-\kappa t}$ that holds [3,4] for a thermally activated exit over an energy barrier of height ΔE such that $\Delta E \gg k_B T$, where T is temperature and k_B is the Boltzman constant. In this limit $\kappa \propto \exp(-\Delta E/k_B T)$, and the thermal relaxation rate is identified with the first nonzero eigenvalue [5,6] of the Fokker-Planck equation, $\kappa=-\lambda_1 \ll -\lambda_n$ for $n \geq 2$. At very short times $t \ll \kappa^{-1}$ the relaxing system is assumed to undergo a local equilibrization (governed by the higher eigenvalues) and the exit process (governed by λ_1) commences only after a local quasistationary state has been established [1]. The initial state of the relaxing system is irrelevant.

Deviations from exponential decay are to be expected, in particular, at large biasing fields, which lower the barrier height ΔE. These non-Markovian processes have been, to date, studied mostly by means of numerical simulations (see, e.g., Ref. [7]). Recently, however, Coffey *et al.* [8] made use of the fact that Brown's Fokker-Planck equation for an axially symmetric system depends on only one phase-space variable and derived semianalytic expressions for correlation functions of a thermally relaxing uniaxial particle. The method of Coffey *et al.* is based on a continued fraction expansion formalism. We proffer here an alternate treatment, based on the so-called shooting method of adjoints [9,10], and express the decay law $W(t)$ in terms of a solution of a Volterra integral equation. A particularly simple result, discussed here in some detail, is obtained if backscattering is neglected; a somewhat more complicated expression holds if backscattering is taken into account.

We assume coherent rotation of magnetization and consider a uniaxial particle with saturation magnetization M_s, anisotropy constant K, and nucleation field $H_n=2K/M_s$. The particle is subject to an external magnetic field H applied parallel to its easy axis, and for its energy we write [2]

$$E=K(1-x^2-2hx), \tag{1}$$

where $h=H/H_n$ is the reduced applied field, $x=\cos\vartheta$, and the angle ϑ is spanned by the easy axis and the magnetization vector $\vec{M}$, $|\vec{M}|=M_s$. The corresponding Fokker-Planck equation has the simple form [2,5,8]

$$\frac{\partial P}{\partial \tau}=\frac{\partial}{\partial x}(1-x^2)\left(-x-h+\sigma\frac{\partial}{\partial x}\right)P, \tag{2}$$

where the reduced temperature $\sigma=k_B T/2K$ and the reduced time $\tau=2\eta K t$; η is a dissipation constant and $P=P(x,\tau)$ is the normalized probability distribution of the magnetization vector orientation.

II. THE REVERSAL TIMES DISTRIBUTION

For definitness we shall now assume that the applied field $h\in\langle 0,1)$, so that the energy (1) has a local maximum at the point $x_0=-h\leq 0$, and two local minima at $x_\pm=\pm 1$. We further assume that at time $t=0$ the particle is in the less stable "down" state, i.e., that the initial distribution $P(x,0)$ is localized within the interval $(-1,-h)$. The problem is that of finding the probability,

$$W_1(t)=\int_{-1}^{-h}dx\,P(x,t), \tag{3}$$

$W_1(0)=1$, that the particle is in the "down" state at $t>0$. Ignoring backscattering we impose on the distribution function $P(x,\tau)$ the absorbing boundary condition $P(-h,\tau)=0$ and write [4]

$$\frac{dW_1(\tau)}{d\tau}=\sigma(1-h^2)\frac{\partial P(x,\tau)}{\partial x}\bigg|_{x=-h}\overset{\text{def}}{=}-Q_1(\tau), \tag{4}$$

by virtue of Eq. (2). The distribution of exit times $Q(\tau)$ is thus fully determined by the single derivative $\partial P/\partial x|_{x=-h}$.

We calculate the Laplace transform of $\hat{Q}_1(z)$, together with its residues, using the shooting method of adjoints [9,10]. In order to implement this method we take the Laplace transform of the Fokker-Planck equation (2), define the quantities

$$y_1(x,z)=(1-x^2)\hat{P}'(x,z), \tag{5}$$

$$y_2(x,z)=\hat{P}(x,z), \tag{6}$$

and $\hat{P}'=d\hat{P}/dx$, and write the transformed Eq. (2) as

$$\sigma\frac{d}{dx}\begin{pmatrix}y_1\\y_2\end{pmatrix}=A\begin{pmatrix}y_1\\y_2\end{pmatrix}-P(x,0)\begin{pmatrix}1\\0\end{pmatrix}, \tag{7}$$

where the matrix $A=A(x,z)$ is

$$A=\begin{pmatrix}x+h & z-2x(x+h)+1-x^2\\ \sigma/(1-x^2) & 0\end{pmatrix}. \tag{8}$$

Equation (7) is to be solved with the natural boundary condition $y_1(-1,z)=0$ and the absorbing boundary condition $y_2(-h,z)=0$. The other two boundary conditions, for the as yet undetermined quantities $y_1(-h,z)$ and $y_2(-1,z)$, follow from the identity [9]

$$y_2(-1)\xi_2(-1)-y_1(-h)\xi_1(-h)=\frac{1}{\sigma}\int_{-1}^{-h}dx\,P(x,0)\xi_1(x), \tag{9}$$

where the functions $\xi_i(x,z)$ satisfy the adjoint equation,

$$\sigma\frac{d}{dx}\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix}=-A^T\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix}, \tag{10}$$

and A^T is the transpose of the matrix A. According to Eqs. (4) and (5) the quantity of interest is the function $y_1(-h,z)$, and in order to find it we impose on the adjoint equation (10) the initial conditions $\xi_1(-1,z)=1$ and $\xi_2(-1,z)=0$ with which the identity (9) yields

$$\hat{Q}_1(z)=\frac{1}{\xi_1(-h,z)}\int_{-1}^{-h}dx\,P(x,0)\xi_1(x,z). \tag{11}$$

This simple formula, expressesing the switching times distribution in terms of the initial probability distribution $P(x,0)$, is the central result of the present paper. We note that both the numerator and the denominator of the right-hand side are regular functions of z so that the poles of $\hat{Q}_1(z)$ coincide with the zeroes of $\xi_1(-h,z)$.

According to Eq. (10) the desired function $\xi_1(x,z)$ satisfies the Volterra integral equation,

$$\xi_1(x)=e^{\varepsilon(x)-\varepsilon(-1)}+\frac{e^{\varepsilon(x)}}{\sigma}\int_{-1}^{x}dx_1\frac{e^{-\varepsilon(x_1)}}{1-x_1^2}\times\int_{-1}^{x_1}dx_2[z-2x_2(x_2+h)+1-x_2^2]\xi_1(x_2), \tag{12}$$

where $\varepsilon(x)=-(x^2+2hx)/2\sigma$ is, up to an additive constant, the reduced energy E/k_BT. With our choice of $P(x,0)$ the reduced height of the barrier to be overcome by thermal activation is $\Delta E/k_BT=(1-h)^2/2\sigma$. Reversals in the opposite direction are here excluded.

In order to solve Eq. (12) we divide the interval $\langle -1,-h\rangle$ into N equal subintervals of length $\Delta=(1-h)/N$, define the function $\xi_1(x)$ by the set of $N+1$ values $\xi_1(x^{(n)})$, $n=0,1,\ldots,N$, at the points $x^{(n)}=-1+n\Delta$, and seek then these values using numerical Picard iterations [10,11]. The inner intergration over x_2 is easily done using the trapezoidal rule, but the outer integral over x_1 has a weak (removable) singularity at $x_1=-1$, and we adopt here a piece-wise linear approximation only for the regular part of the integrand.

If the function $\xi_1(x,z)$ is known, then formal differentiation of Eq. (12) with respect to z yields a weakly singular Volterra integral equation for the function $\partial\xi_1(x,z)/\partial z$ that determines, by virtue of Eq. (11), the residues of the reversal times distribution $\hat{Q}_1(z)$. The function $\xi_1(-h,z)$ has infinitely many simple roots $z^{(i)}$ along the negative real axis of the complex z plane, and in the vicinity of the ith root we write $\xi_1(-h,z)\approx(z-z^{(i)})\partial\xi_1(-h,z^{(i)})/\partial z$.

III. DECAY LAW

Equation (11) makes it possible to study the decay of an arbitrary initial state. We chose here the simple singular [12] initial distribution $P(x,0)=\delta(x+1)$ for which $\hat{Q}_1(z)\xi_1(-h,z)=1$. Sample plots of this function $\hat{Q}_1(z)$ are shown in Figs. 1 and 2. In plotting these figures we scaled the real axis of the complex z plane, introducing the notation,

$$\rho(z)=\begin{cases}(z\Upsilon)^{1/2} & \text{if } z\geqslant 0\\ -(-z\Upsilon)^{1/2} & \text{if } z\leqslant 0,\end{cases} \tag{13}$$

and the mean first passage time,

$$\Upsilon=\int_{-1}^{-h}\frac{dx_1\,e^{\varepsilon(x_1)}}{1-x_1^2}\int_{-1}^{x_1}dx_2\,e^{-\varepsilon(x_2)}. \tag{14}$$

Within this scale the poles of $\hat{Q}_1(z)$ are almost equidistant.

For $P(x,0)=\delta(x+1)$ and $\xi_1(-1,z)=1$ the real time exit times distribution $Q_1(\tau)$ is given by the equation,

$$Q_1(\tau)=\sum_i\left(\frac{\partial\xi_1(-h,z^{(i)})}{\partial z}\right)^{-1}\exp(\tau z^{(i)}), \tag{15}$$

and the normalization of $Q_1(\tau)$ then serves as an independent check on the numerical accuracy of the computation. The probability $W_1(\tau)$ that the particle has not reversed at the time $\tau\geqslant 0$ then follows, and we plot a sample family of these curves in Fig. 3. The low-temperature exponential decay is defined by the Markovian limit, and for this reason we concentrate here on the opposite limit of high temperatures and set $\sigma=1$. A striking feature of the shown plots is the very slow initial decay at short times. This is characteristic of processes in which the initial distribution is negligibly small close to the top of the barrier; the slow initial phase of the decay here corresponds to initial equilibrization *within* the well [13]. By contrast, the initial decay is faster than the exponential limit [dashed line in Fig. 3] if at $\tau=0$ there is an appreciable probability of finding the system close to the top of the barrier (not shown).

IV. CONCLUDING REMARKS

The right-hand side of the Fokker-Planck equation has the form of a divergence of a probability current $\vec{J}$, and it is, therefore, possible to relate the decay law $W(t)$ to values, which the distribution function $P(x,t)$ takes on at the edges

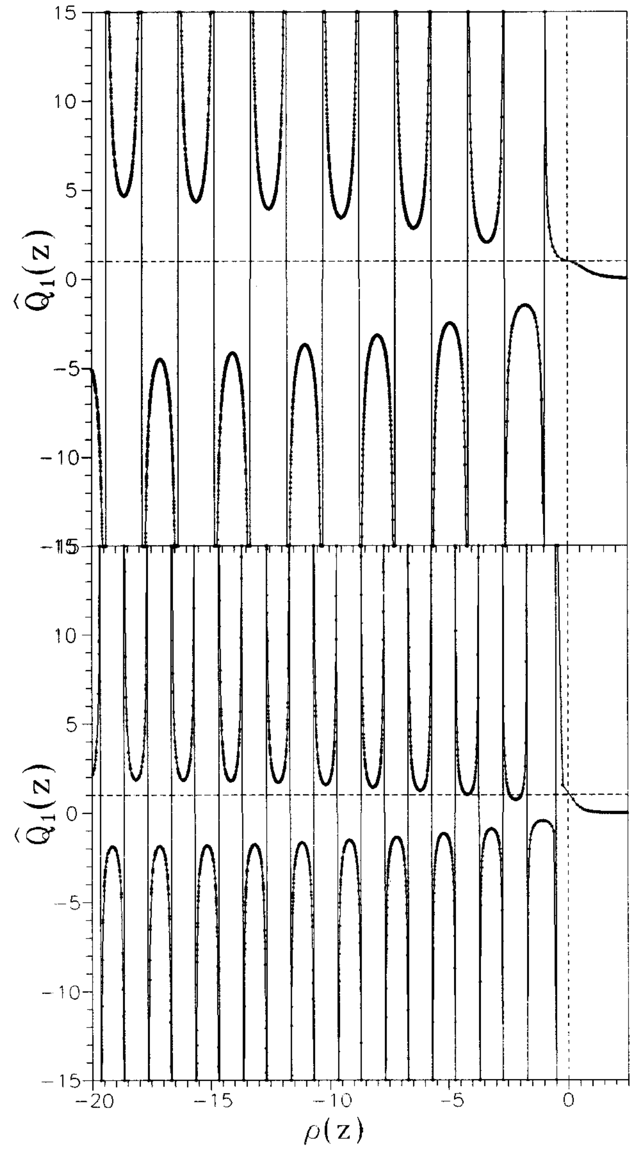

FIG. 1. The function $\hat{Q}_1(z)$ along the scaled [see Eq. (13)] real axis of the complex z plane. Reduced applied field $h=0$ and reduced temperature $\sigma=1$ [top, with $\Upsilon\approx0.579$] and $\sigma=0.2$ [bottom, with $\Upsilon\approx1.232$]. $\hat{Q}_1(0)=1$ by virtue of the normalization $W(0)_1=1$.

of a one-dimensional metastable domain. We have chosen to treat here Brown's Fokker-Planck equation because of its relation to recent experimental works [13], but the proposed method is equally well applicable also to the Smoluchowski equation and to its various generalizations [14]. In particular, for an overdamped Brownian particle driven by white noise, the probability current $J=\eta[V'(x)+k_BT\partial/\partial x]P$ leads to a very simple adjoint system whose numerical solution is almost trivial for any potential $V=V(x)$.

The formalism presented so far has the drawback of being restricted to thermal decay of a *single* metastable state. In this concluding section we abandon the absorbing boundary condition $P(-h,t)=0$ and outline the somewhat more elaborate treatment of the thermally relaxing *bistable* system described by Eqs. (1) and (2).

In analogy to Eq. (3) we define in this case also the probability

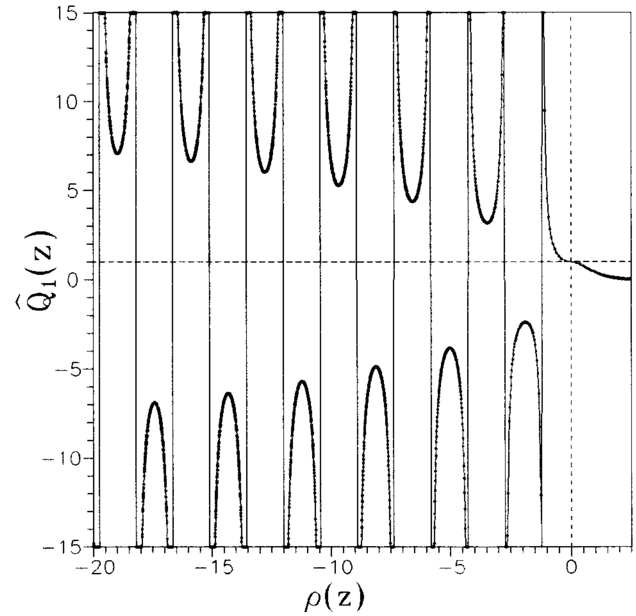

FIG. 2. The function $\hat{Q}_1(z)$ along the scaled [see Eq. (13)] real axis of the complex z plane. Reduced applied field $h=0.8$ and reduced temperature $\sigma=1$; $\Upsilon\approx0.101$.

$$W_2(t)=\int_{-h}^{1}dx\,P(x,t), \tag{16}$$

$W_1(t)+W_2(t)\equiv1$, that the particle is in the ''up'' state, and write then the modified Eq. (4) in the form,

$$\dot{W}_1(\tau)=-\dot{W}_2(\tau)\overset{\text{def}}{=}-Q_1(\tau)$$
$$=\sigma(1-h^2)P'(-h,\tau), \tag{17}$$

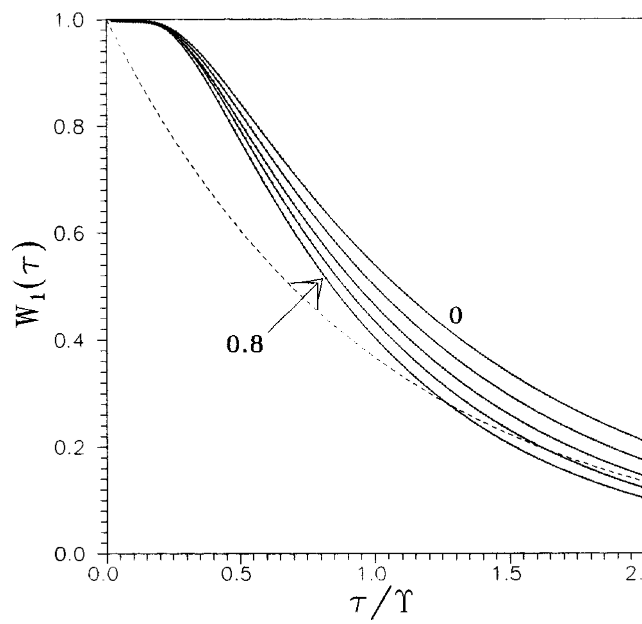

FIG. 3. The probability $W_1(\tau)$ of finding the particle in the ''down'' state (solid lines) versus the reduced time τ/Υ. Reduced applied field consecutively $h=0$ (labeled), 0.2, 0.4, 0.6, and 0.8 (labeled), and reduced temperature $\sigma=1$. The dashed line represents exponential decay.

$\dot{W}_i = dW_i/d\tau$. In place of Eq. (9) we now have [9]

$$y_1(-h)\xi_1^{(i)}(-h)+y_2(-h)\xi_2^{(i)}(-h)-y_2(-1)\xi_2^{(i)}(-1) = -\frac{1}{\sigma}\int_{-1}^{-h} dx\, P(x,0)\xi_1^{(i)}(x), \quad (18)$$

$i=1$ and 2, where the functions $\xi_1^{(i)}$ and $\xi_2^{(i)}$ are two solutions of the adjoint equation (10) on the interval $(-1,-h\rangle$. Similarly, on the interval $\langle -h,1)$, there is

$$y_2(1)\xi_2^{(i)}(1)-y_1(-h)\xi_1^{(i)}(-h)-y_2(-h)\xi_2^{(i)}(-h) = -\frac{1}{\sigma}\int_{-h}^{1} dx\, P(x,0)\xi_1^{(i)}(x), \quad (19)$$

and with a suitable choice of initial (final) conditions imposed on Eq. (10) the four equations (18) and (19) constitute a linear system for the four unknowns $y_2(-1)$, $y_1(-h)$, $y_2(-h)$, and $y_2(1)$. A convenient choice is $\vec{\xi}^{(1)}(-h)=(1,0)$ and $\vec{\xi}^{(2)}(-h)=(0,1)$ for which one obtains two solutions of Eq. (10), which are continuous on the entire interval $(-1,1)$. With this choice the poles of the Laplace transformed probabilities $\hat{W}_i(z)$ coincide with the zeroes of the function,

$$\mathcal{D}(z) = z\det\begin{pmatrix} \xi_2^{(1)}(-1,z) & \xi_2^{(1)}(1,z) \\ \xi_2^{(2)}(-1,z) & \xi_2^{(2)}(1,z) \end{pmatrix}, \quad (20)$$

and we note that the pole at $z=0$ then corresponds to the state of thermal equilibrium; in the preceding case, where $\lim_{t\to\infty} W_1(t)=0$ due to the absence of backscattering, this pole canceled identically.

In summary, using the shooting method of adjoints we have reduced the one-dimensional Fokker-Planck equation to an expression for a finite number of the discrete occupation probabilities $W_i(t)$.

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