

Evaluation of the smallest nonvanishing eigenvalue of the Fokker-Planck equation for the Brownian motion in a potential. II. The matrix continued fraction approach

Yu. P. Kalmykov

Centre d'Études Fondamentales, Université de Perpignan, 52 Avenue de Villeneuve, 66860 Perpignan Cedex, France

(Received 21 March 2000)

An equation for the smallest nonvanishing eigenvalue λ_1 of the Fokker-Planck equation (FPE) for the Brownian motion of a particle in a potential is derived in terms of matrix-continued fractions. This equation is applicable to the calculation λ_1 if the solution of the FPE can be reduced (by expanding the probability distribution function in terms of a complete set of appropriate functions) to the solution of a multiterm recurrence relation for the moments describing the dynamics of the Brownian particle. In contrast to the available continued fraction solution for λ_1 [H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1989)], this equation does not require one to solve numerically a high order polynomial equation. To test the theory, the smallest eigenvalue λ_1 is evaluated for the FPE, which appears in the theory of magnetic relaxation of single domain (superparamagnetic) particles. Various regimes of relaxation of the magnetization in superparamagnetic particles are governed by a damping parameter α , the limiting values of which correspond to the high damping ($\alpha \rightarrow \infty$) and the low damping ($\alpha \ll 1$) limits in the theory of the escape rate over potential barriers. It is shown that for all ranges of the barrier height and damping parameters the smallest eigenvalue λ_1 predicted by the continued fraction equation is in agreement with those gained by independent numerical methods and the asymptotic estimates for λ_1 (in the high barrier limit) and, moreover, the matrix continued fraction approach may be successfully applied to the evaluation of λ_1 in those ranges of parameters where traditional methods fail or are not applicable.

PACS number(s): 05.40.Jc, 05.10.Gg, 75.50.Tt

I. INTRODUCTION

In the previous paper [1], we elaborated on a method used to calculate the smallest nonvanishing eigenvalue λ_1 of the FPE for the Brownian motion of a particle in a potential, where the dynamics of the system is governed by an infinite hierarchy of *scalar three-term* recurrence equations for the moments (the expectation values of the dynamic quantities of interest). As is well known [2,3], for the majority of problems the FPE may not be reduced to the solution of a scalar three-term recurrence equation. Hence the method [1] of evaluating λ_1 based on the conversion of the recurrence relation to ordinary continued fractions can no longer be applicable. Examples of this are those problems, which involve diffusion in phase space and diffusion in configuration space where the form of a potential is such as to give rise to multiterm recurrence relations. In the present paper, the method [1] is extended for *multiterm* recurrence equations, which can be solved in terms of matrix-continued fractions [2,3].

As is known [2], a *multiterm scalar* recurrence relation may be converted to a *three-term matrix* one. Such a matrix three-term recurrence relation may be written down as

$$\tau_e \frac{d}{dt} \mathbf{C}_n(t) = \mathbf{Q}_n^- \mathbf{C}_{n-1}(t) + \mathbf{Q}_n \mathbf{C}_n(t) + \mathbf{Q}_n^+ \mathbf{C}_{n+1}(t),$$

$$n = 1, 2, 3, \dots \tag{1}$$

where the $\mathbf{C}_n(t)$ are the column vectors arranged from the moments in an appropriate way. \mathbf{Q}_n^- , \mathbf{Q}_n^+ , and \mathbf{Q}_n are time independent noncommutative matrices, and τ_e is a characteristic time constant. A general method used to solve Eq. (1) in terms of matrix continued fractions has been described by Risken [2] and later extended by Coffey *et al.* [3]. According to [3], the *exact solution* of Eq. (1) with $\mathbf{C}_0(t) = \mathbf{0}$ for the Laplace transform of $\mathbf{C}_1(t)$ is given by

$$\tilde{\mathbf{C}}_1(s) = \tau_e \Delta_1(s) \left\{ \mathbf{C}_1(0) + \sum_{n=2}^{\infty} \left[\prod_{k=2}^n \mathbf{Q}_{k-1}^+ \Delta_k(s) \right] \mathbf{C}_n(0) \right\},$$

$$\tag{2}$$

where the infinite matrix continued fraction $\Delta_n(s)$ is defined as

$$\Delta_n(s) = \frac{\mathbf{I}}{\tau_e s \mathbf{I} - \mathbf{Q}_n - \mathbf{Q}_n^+ \frac{\mathbf{I}}{\tau_e s \mathbf{I} - \mathbf{Q}_{n+1} - \mathbf{Q}_{n+1}^+ \frac{\mathbf{I}}{\tau_e s \mathbf{I} - \mathbf{Q}_{n+2} - \dots \mathbf{Q}_{n+2}^-} \mathbf{Q}_{n+1}^-} \mathbf{Q}_{n+1}^-} \mathbf{I} \tag{3}$$

(the fraction lines designate the matrix inversions) and \mathbf{I} is the unit matrix. The initial conditions $\mathbf{C}_p(0)$ in Eq. (2) can be expressed in terms of the matrix continued fraction $\Delta_p(0)$ (see, e.g., Refs. [2,3]).

Having determined the Laplace transform $\tilde{\mathbf{C}}_1(s)$ from Eq. (2), one is able to calculate the relaxation time τ_k of the k th component $c_{1,k}(t)$ of $\mathbf{C}_1(t)$, which is defined as

$$\tau_k = \frac{1}{c_{1,k}(0)} \int_0^\infty c_{1,k}(t) dt = \frac{\tilde{c}_{1,k}(0)}{c_{1,k}(0)}. \quad (4)$$

The relaxation time τ_k may equivalently be defined in the context of the FPE converted to the Sturm-Liouville problem as

$$\tau_k = \frac{\sum_m C_{km} / \lambda_{km}}{\sum_m C_{km}}, \quad (5)$$

where λ_{km} and C_{km} are the eigenvalues and their corresponding weight coefficients (amplitudes), as

$$c_{1,k}(t) = \sum_m C_{km} e^{-\lambda_{km} t}. \quad (6)$$

The relaxation time τ_k Eq. (5) contains contributions from *all* the eigenvalues. In general, it is impossible to evaluate τ_k analytically from Eq. (6) as knowledge of all λ_{km} and C_{km} is required. As far as a physical interpretation is concerned, in many cases the relaxation time τ_k is determined by the slowest low-frequency relaxation mode that governs transitions of the Brownian particle over the barriers from one potential well into another. The characteristic frequency of this over-barrier relaxation mode is determined by the smallest eigenvalue λ_1 . It is apparent from Eq. (6) that λ_1 is the reciprocal time constant associated with the *long time behavior* of the relaxation function, which is only determined by the slowest low-frequency relaxation mode. The behavior of the relaxation time and the inverse of the smallest eigenvalue λ_1 is sometimes similar. However, if different time scales are involved, the behavior of these can be quite different. An example of this is the Brownian motion of a particle in a bistable potential under the action of a constant field [4], where the relaxation time may *diverge exponentially* from the inverse of the smallest nonvanishing eigenvalue λ_1 . Here for moderate values of the constant field a close approximation to the correlation time is furnished by λ_1^{-1} ; however, as the field strength increases so that the bistable nature of the potential is weakened, λ_1^{-1} ceases to be a good approximation for the relaxation time (see Sec. III). A knowledge of λ_1 is also of importance because other time constants, such as the mean first passage time and the escape rate, are mainly determined by the slowest low-frequency relaxation mode. Moreover, in many cases the influence of other relaxation modes in the low-frequency relaxation may be ignored and, thus, the knowledge of λ_1 provides sufficient information about the low-frequency dynamics of the system [2].

The continued fraction approach of calculating the eigenvalues of the FPE has been discussed in detail by Risken [2].

In Ref. [1] we further developed this approach and suggested a usable method for evaluating the smallest nonvanishing eigenvalue λ_1 of the FPE in terms of scalar continued fractions. In contrast to the previously available solution [2], the method developed does not require one to solve numerically a high order polynomial equation as it was shown that λ_1 may be represented as a sum of products of infinite continued fractions. Besides its advantage for the numerical calculation, the equation so obtained is very useful for analytical purposes, e.g., for certain problems it may be expressed in terms of known mathematical (special) functions.

Here we extend the method of Ref. [1] to the problem under consideration. We consider as an example of the applicability of the method the problem of magnetic relaxation of single domain particles. A single domain particle is characterized by an internal potential, which can have several local states of equilibrium with potential barriers between them. If the particles are small (~ 10 nm) so that the potential barriers are relatively low, the magnetization vector \mathbf{M} may cross over the barriers between one potential well and another due to thermal agitation. The ensuing thermal instability of magnetization results in the phenomenon of superparamagnetism [5]. The thermal fluctuations and relaxation of the magnetization of superparamagnetic particles currently merit attention in view of their importance in the context of magnetic recording media and rock magnetism, as well as in connection with the observation of magnetization reversal in isolated ferromagnetic nanoparticles and nanowires [6].

The thermal fluctuations of the magnetization \mathbf{M} in an individual superparamagnetic particle are described by the FPE for the probability density distribution W of \mathbf{M} [7]:

$$2\tau_N \frac{\partial}{\partial t} W = \beta [\alpha^{-1} \mathbf{u} \cdot (\text{grad } V \times \text{grad } W) + \text{div}(W \text{ grad } V)] + \Delta W, \quad (7)$$

where Δ is the Laplacian on the surface of the unit sphere, \mathbf{u} is the unit vector directed along \mathbf{M} , V is the free energy density of the magnetocrystalline anisotropy expressed as a function of \mathbf{M} ,

$$\tau_N = \beta \eta M_s^2 (1 + \alpha^{-2}) / 2 \quad (8)$$

is the characteristic relaxation time, $\beta = \nu / kT$, ν is the volume of the particle, k is the Boltzmann constant, T is the temperature, γ is the gyromagnetic ratio, η is the damping parameter. M_s is the saturation magnetization, and $\alpha = \gamma \eta M_s$ is the dimensionless dissipation parameter. A discussion of the assumptions made in the derivation of the FPE (7) is given elsewhere (e.g., [8,9]). It is of importance that the general theory of the escape rates over the potential barriers [10] has a direct application to the present problem [11]. Various regimes of relaxation of superparamagnetic particles are governed by the damping parameter α , the intermediate and large ($1 \leq \alpha \leq \infty$) and small ($\alpha \ll 1$) values of which correspond to the intermediate to high damping and the low damping limits of the escape rate theory [10,11]. For $\alpha = \infty$ the FPE (7) is similar to that for the rotational Brownian motion of a particle in a liquid [3].

A standard approach to the solution of Eq. (7) is to expand the probability distribution function W in terms of spherical harmonics $Y_{l,m}$ defined as [12]

$$Y_{l,m} = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\varphi} P_l^m(\cos \vartheta),$$

$$Y_{l,-m} = (-1)^m Y_{l,m}^*, \quad (9)$$

where $P_l^m(\cos \vartheta)$ is the associated Legendre function, and the asterisk denotes the complex conjugate. This yields an infinite hierarchy of differential-recurrence equations for the moments $c_{l,m}(t)$ (the expectation values of the spherical harmonics or appropriate correlation functions) [13,14]:

$$\tau_N \frac{d}{dt} c_{l,m}(t) = \sum_{l',m'} d_{l',m',l,m} c_{l',m'}(t), \quad (10)$$

where $d_{l',m',l,m}$ are the matrix elements of the Fokker-Planck operator [14]: $d_{l',m',l,m}$ depend on parameters characterizing the anisotropy energy, external fields, and dissipation. An equation for $d_{l',m',l,m}$ at an arbitrary V was derived in [13]. Equation (10) may be reduced to Eq. (1) by means of the appropriate arrangement of the column vectors $\mathbf{C}_n(t)$ and the matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- (see, for example, Ref. [15]).

The paper is arranged as follows. In Sec. II, an equation for the smallest eigenvalue λ_1 is derived in terms of matrix-continued fractions. The verification of the validity of this equation is given in Secs. III and IV by evaluating λ_1 for the FPE for the Brownian motion of a particle in asymmetric bistable potentials, which appears in the theory of superparamagnetism.

II. MATRIX-CONTINUED FRACTION SOLUTION FOR λ_1

In the context of the matrix continued fraction approach, the eigenvalues of the FPE can be determined by inserting the separation ‘‘ansatz’’ [2]

$$\mathbf{C}_n(t) = \hat{\mathbf{C}}_n e^{-\lambda t}, \quad n = 1, 2, 3, \dots \quad (11)$$

into Eq. (1). Thus one can obtain an equation for the eigenvalues, viz,

$$\det[\tau_\varepsilon \lambda \mathbf{I} + \mathbf{Q}_1 + \mathbf{Q}_1^+ \Delta_2(-\lambda) \mathbf{Q}_2^-] = 0. \quad (12)$$

The disadvantage of Eq. (12) is that in some cases it may be extremely difficult to evaluate eigenvalues as it involves finding the roots of a very high order polynomial equation. The direct matrix methods, which are based on writing the set of the moment equations (10) as a first-order matrix differential equation,

$$\frac{d}{dt} \mathbf{X}(t) = \mathbf{A} \mathbf{X}(t), \quad (13)$$

and on subsequent numerical solutions of Eq. (13), may also be inapplicable in those limits, as it is necessary to carry out the calculations for the dimension of the column vector $\mathbf{X}(t)$ of the order of 10^4 - 10^5 , and convergence of the solution is consequently difficult to achieve [16].

Equation (12) allows one to evaluate numerically all the eigenvalues [2]. However, if one is interested in the evaluation of λ_1 only, Eq. (12) can be simplified just as for the scalar continued fraction [1]. In the high barrier (or low temperature) limit, where $\tau_\varepsilon \lambda_1 \ll 1$ [2], one may take into account only the first two terms in the Taylor series expansion of $\Delta_2(-\lambda)$ for $\lambda = \lambda_1$, viz,

$$\Delta_2(-\lambda_1) = \Delta_2(0) - \lambda_1 \tau_\varepsilon \Delta_2'(0) + O((\lambda_1 \tau_\varepsilon)^2). \quad (14)$$

Thus one has from Eq. (12)

$$\det[\tau_\varepsilon \lambda_1 \{\mathbf{I} - \mathbf{Q}_1^+ \Delta_2'(0) \mathbf{Q}_2^-\} + \mathbf{Q}_1 + \mathbf{Q}_1^+ \Delta_2(0) \mathbf{Q}_2^-] = 0, \quad (15)$$

where the symbol ' designates the derivative of $\Delta_2(s)$ with respect to $s \tau_\varepsilon$. As will be shown below, Eqs. (14) and (15) also provide relatively high accuracy in the calculation of λ_1 for intermediate and small barrier heights, where $\tau_\varepsilon \lambda_1 \leq 1$. In order to calculate λ_1 from Eq. (15), one should obtain an equation for $\Delta_2'(0)$. This can be accomplished by noting that $\Delta_n(s)$ and $\Delta_n'(s)$ satisfy the following recurrence relations:

$$\Delta_n(s) = [\tau_\varepsilon s \mathbf{I} - \mathbf{Q}_n - \mathbf{Q}_n^+ \Delta_{n+1}(s) \mathbf{Q}_{n+1}^-]^{-1} \quad (16)$$

and

$$\Delta_n'(s) = -[\mathbf{I} - \mathbf{Q}_n^+ \Delta_{n+1}'(s) \mathbf{Q}_{n+1}^-] \Delta_n^2(s), \quad (17)$$

respectively [Eq. (17) can be obtained by direct differentiation of Eq. (16)]. Equation (17) can be further rearranged in the form of the recurrence equation for $\mathbf{Q}_{n-1}^+ \Delta_n'(s) \mathbf{Q}_n^-$, viz,

$$\mathbf{Q}_{n-1}^+ \Delta_n'(s) \mathbf{Q}_n^- = -\mathbf{Q}_{n-1}^+ [\mathbf{I} - \mathbf{Q}_n^+ \Delta_{n+1}'(s) \mathbf{Q}_{n+1}^-] \Delta_n^2(s) \mathbf{Q}_n^-,$$

the solution of which may be obtained by iteration and is given by, for $s=0$,

$$\mathbf{Q}_1^+ \Delta_2'(0) \mathbf{Q}_2^- = - \sum_{n=2}^{\infty} \left(\prod_{m=1}^{n-1} \mathbf{Q}_m^+ \right) \times \left(\prod_{k=1}^{n-1} \Delta_{n-k+1}^2(0) \mathbf{Q}_{n-k+1}^- \right). \quad (18)$$

Thus the substitution of Eq. (18) into Eq. (15) yields

$$\det(\lambda_1 \mathbf{I} - \mathbf{S}) = 0, \quad (19)$$

where the matrix \mathbf{S} is defined as

$$\mathbf{S} = -\tau_\varepsilon^{-1} [\mathbf{Q}_1 + \mathbf{Q}_1^+ \Delta_2(0) \mathbf{Q}_2^-] \left[\mathbf{I} + \sum_{n=2}^{\infty} \left(\prod_{m=1}^{n-1} \mathbf{Q}_m^+ \right) \times \left(\prod_{k=1}^{n-1} \Delta_{n-k+1}^2(0) \mathbf{Q}_{n-k+1}^- \right) \right]^{-1}. \quad (20)$$

Here, we have made use of a theorem ([17], Sec. 14.8-7), which states that the eigenvalues μ and eigenvectors \mathbf{y} of the matrix equation

$$\mathbf{A} \mathbf{y} = \mu \mathbf{B} \mathbf{y}$$

are the eigenvalues and eigenvectors of the matrix $\mathbf{B}^{-1}\mathbf{A}$. Thus the smallest nonvanishing eigenvalue λ_1 is an eigenvalue of the matrix \mathbf{S} given by Eq. (20). Furthermore, if that $\lambda_1 \ll \lambda_n$ (λ_n are all other eigenvalues of the matrix \mathbf{S}), then λ_1 is given by

$$\lambda_1 \approx \frac{\det[\mathbf{S}]}{\text{Sp}[\mathbf{D}]}, \quad (21)$$

where the elements of the matrix \mathbf{D} are the minors of the matrix \mathbf{S} . The evaluation of λ_1 from Eq. (19) or Eq. (21) is much more easily accomplished than the calculation of λ_1 by solving numerically a high order polynomial Eq. (12) or by using the matrix Eq. (13). Equation (19) requires only the calculation of the matrix-continued fractions $\Delta_n(0)$.

III. APPLICATIONS TO RELAXATION PROBLEMS OF SUPERPARAMAGNETISM: BIASED UNIAXIAL POTENTIAL

As an example let us consider a uniaxial superparamagnetic particle in a strong uniform magnetic field \mathbf{H}_0 applied along the easy axis. Here, the anisotropy energy density is given by [18–20]

$$V = -K \cos^2 \vartheta - H_0 M_s \cos \vartheta, \quad (22)$$

where K is the anisotropy constant and ϑ is the angle between \mathbf{M} and the positive z axis. Similar problems related to the rotational Brownian motion in potential (22) also appear in the theory of dielectric relaxation of nematic liquid crystals [21] and the theory of the dynamic Kerr effect [22]. In the theory of superparamagnetism, the potential (22) was originally introduced by Néel [23], who gave an expression for the time of reversal of the magnetization. It was further considered by Brown [24], who obtained approximate expressions for the lowest eigenvalue in the limit of large and small K using the Kramers transition state method [25] and perturbation theory, respectively. Later, the smallest eigenvalue λ_1 was calculated numerically by Aharoni [18]. On the other hand, the analysis presented by Garanin *et al.* [19,26] enabled them to derive an integral expression for the longitudinal relaxation time τ from the FPE (7). The relaxation time τ has also been calculated using the matrix-continued fraction approach [27], where the bias field effect of the exponential deviation of τ from the inverse of λ_1 has been discovered. Here we apply the matrix-continued fraction technique to the calculation of λ_1 . The model is used here as an example to verify the continued fraction solution Eq. (19).

Furthermore, although this model has already been studied in Refs. [18,24,27], an equation for λ_1 , however, which would be valid for all ranges of the barrier heights, has not yet been presented. The continued fraction solution Eq. (19) will be compared with the asymptotic solution of Brown [24] for λ_1 in the high barrier limit and the solution of Garanin [26] and Coffey *et al.* [27] for the longitudinal relaxation time.

Upon evaluating the longitudinal relaxation of the particle, the FPE (7) with the potential (22) can be reduced [27] to the solution of the infinite hierarchy of five-term recurrence equations for the equilibrium correlation functions $f_n(t)$, which describes the dynamics of the system under consideration, viz,

$$\begin{aligned} & \frac{2\tau_N}{n(n+1)} \frac{d}{dt} f_n(t) + \left[1 - \frac{2\sigma}{(2n-1)(2n+3)} \right] f_n(t) \\ &= \frac{\xi}{2n+1} [f_{n-1}(t) - f_{n+1}(t)] \\ &+ 2\sigma \left[\frac{(n-1)}{(2n-1)(2n+1)} f_{n-2}(t) \right. \\ &\left. - \frac{(n+2)}{(2n+1)(2n+3)} f_{n+2}(t) \right], \quad (23) \end{aligned}$$

where

$$\begin{aligned} f_n(t) &= \langle \cos \vartheta(0) P_n[\cos \vartheta(t)] \rangle_0 \\ &- \langle \cos \vartheta(0) \rangle_0 \langle P_n[\cos \vartheta(0)] \rangle_0, \\ \sigma &= \frac{\nu K}{kT}, \quad \xi = \frac{\nu M_s H_0}{kT} \end{aligned}$$

are the barrier height and the bias field parameters, respectively, P_n are the Legendre polynomials, and $\langle \rangle_0$ designates the equilibrium average at $t=0$.

Equation (23) can be transformed [27] into the matrix three-term differential-recurrence Eq. (1), where $\tau_e = \tau_N$,

$$\mathbf{C}_n(t) = \begin{pmatrix} f_{2n-1}(t) \\ f_{2n}(t) \end{pmatrix}$$

and \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- are the 2×2 matrices given by [27]

$$\mathbf{Q}_n = \begin{pmatrix} \frac{2\sigma n(2n-1)}{(4n-3)(4n+1)} - n(2n-1) & -\xi \frac{n(2n-1)}{4n-1} \\ \xi \frac{n(2n+1)}{4n+1} & \frac{2\sigma n(2n+1)}{(4n-1)(4n+3)} - n(2n+1) \end{pmatrix}, \quad (24)$$

$$\mathbf{Q}_n^+ = \begin{pmatrix} -\sigma \frac{2n(4n^2-1)}{16n^2-1} & 0 \\ -\xi \frac{n(2n+1)}{4n+1} & -\sigma \frac{4n(n+1)(2n+1)}{(4n+1)(4n+3)} \end{pmatrix}. \quad (25)$$

$$\mathbf{Q}_n^- = \begin{pmatrix} \sigma \frac{4n(n-1)(2n-1)}{(4n-1)(4n-3)} & \xi \frac{n(2n-1)}{4n-1} \\ 0 & \sigma \frac{2n(4n^2-1)}{16n^2-1} \end{pmatrix}. \quad (26)$$

The matrix-continued fraction $\Delta_n(0)$ [Eq. (3)] with the 2×2 matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- given by Eqs. (24)–(26) satisfies the conditions of a theorem (proved in Ref. [28]) appropriate to the convergence of matrix-continued fractions. This theorem guarantees the convergence of the matrix-continued fraction $\Delta_n(0)$ defined by Eq. (3) to some limit if two definite conditions are fulfilled, viz,

$$\det[\mathbf{Q}_{n+1}^+(\mathbf{Q}_{n+1})^{-1}] \det[\mathbf{Q}_{n+1}^-(-\mathbf{Q}_n)^{-1}] \leq \frac{1}{4} \text{ for } n > 1$$

and

$$\lim_{N \rightarrow \infty} 4^N \prod_{n=1}^N \det[\mathbf{Q}_{n+1}^+(\mathbf{Q}_{n+1})^{-1}] \det[\mathbf{Q}_{n+1}^-(-\mathbf{Q}_n)^{-1}] = 0. \quad (27)$$

It can be readily verified that the matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- in Eqs. (24)–(26) satisfy the above conditions. Thus the matrix-continued fraction defined by Eq. (3) converges. In our calculation, the infinite matrix-continued fraction $\Delta_n(0)$ was approximated by a matrix-continued fraction of finite order (by putting $\mathbf{Q}_n^+ = \mathbf{0}$ at some $n=N$). The value of N must be chosen by stipulating the accuracy of the calculation *a priori* as it depends on the parameters σ and ξ . The calculation has shown that the matrix-continued fractions and the series involved in Eq. (19) converge very rapidly, thus 10–15 downward iterations in calculating the continued frac-

TABLE I. Numerical values for the biased uniaxial potential Eq. (22) at $h=0.1$

σ	$\tau_N \lambda_1^{\text{num}}$ [Eq. (32)]	$\tau_N \lambda_1$ [Eq. (28)]	$\tau_N \lambda_1^{\text{as}}$ [Eq. (29)]	τ_N / τ [Eq. (30)]
0	1.0	1.0	0.0	1.0
1	0.6569	0.6562	0.4068	0.6587
2	0.4161	0.4151	0.4359	0.4202
3	0.2557	0.25450	0.3146	0.2602
4	0.1530	0.1526	0.1964	0.1566
5	0.0893	0.0891	0.1141	0.0917
6	0.0508	0.0508	0.0636	0.0523
7	0.0283	0.0282	0.0345	0.0291
8	0.0154	0.0154	0.0183	0.0158
9	0.0082	0.0082	0.0096	0.0085
10	0.0043	0.0043	0.0049	0.0045

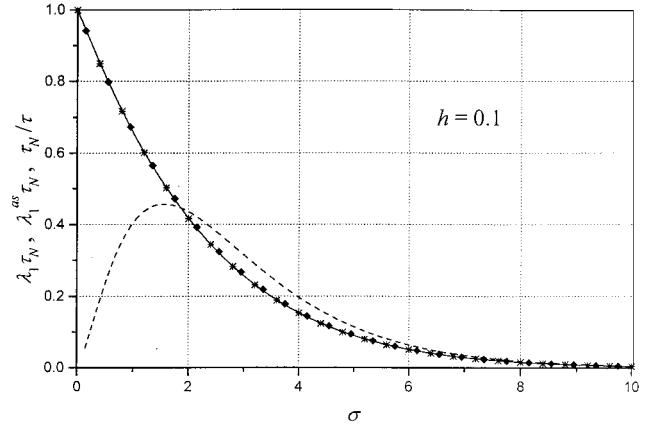


FIG. 1. λ_1 [Eq. (28)—solid line] and λ_1^{num} [Eq. (32)—stars] for the biased $\cos^2 \vartheta$ potential at $h=0.1$ as a function of the barrier height σ compared with the asymptotic solution λ_1^{as} [Eq. (29)] (dashed line) and the solution rendered by the inverse of the correlation time τ^{-1} [Eq. (30)] (diamonds).

tions and 10–15 terms in the series were enough to arrive at an accuracy of not less than six significant digits in the majority of cases.

The smallest nonvanishing eigenvalue λ_1 is determined by Eq. (19). As here the matrix \mathbf{S} in Eq. (19) has the dimension 2×2 , one can readily obtain

$$\lambda_1 = \frac{1}{2} (S_{11} + S_{22} - \sqrt{(S_{11} - S_{22})^2 + 4S_{12}S_{21}}), \quad (28)$$

where S_{ij} are the elements of the matrix \mathbf{S} .

The results of the calculation of λ_1 from Eq. (28) are presented in Table I and Figs. 1 and 2, where they are compared with the asymptotic estimate for λ_1 given by [7,24]

$$\lambda_1^{\text{as}} \sim \frac{\sigma^{3/2}(1-h^2)}{\tau_N \sqrt{\pi}} \{(1+h)e^{-\sigma(1+h)^2} + (1-h)e^{-\sigma(1-h)^2}\}, \quad (29)$$

and with the inverse of the relaxation time τ of the correlation function $f_1(t)$ defined by Eq. (2), which may be equivalently presented in the integral form as [26]

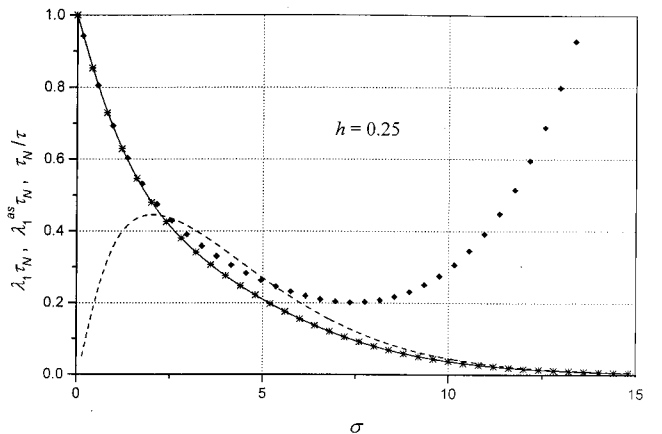


FIG. 2. The same as in Fig. 1 for $h=0.25$.

$$\tau = \frac{2\tau_N}{Z(\langle \cos^2 \vartheta \rangle_0 - \langle \cos \vartheta \rangle_0^2)} \times \int_{-1}^1 \left[\int_{-1}^z (z' - \langle \cos \vartheta \rangle_0) e^{-\beta V(z')} dz' \right]^2 \frac{e^{\beta V(z)}}{1-z^2} dz. \quad (30)$$

Here $h = \xi/2\sigma$,

$$\langle \cos \vartheta \rangle_0 = \frac{1}{Z} \int_{-1}^1 x e^{-\beta V(x)} dx,$$

$$\langle \cos^2 \vartheta \rangle_0 = \frac{1}{Z} \int_{-1}^1 x^2 e^{-\beta V(x)} dx,$$

and

$$\beta V(x) = -\sigma(x^2 + 2hx), \quad Z = \int_{-1}^1 e^{-\beta V(x)} dx. \quad (31)$$

The results of the calculation of λ_1 from Eq. (28) are also compared in Table I with those obtained from the numerical solution of the set of Eq. (23) transformed into the matrix Eq. (13) (see, for details, [27]). The lowest eigenvalue λ_1 is then the smallest root of the characteristic equation

$$\det(\lambda \mathbf{I} - \mathbf{A}) = 0, \quad (32)$$

where \mathbf{A} is a five-diagonal system matrix in Eq. (13), the elements of which are determined by Eq. (23). For the problem in question, the evaluation of λ_1^{num} from Eq. (32) creates no difficulties and it is used here only for the purpose of comparison with the results of the continued fraction approach.

The lowest eigenvalue λ_1 from Eq. (28) is in good agreement with the numerical solutions λ_1^{num} of the characteristic Eq. (32) for all σ (see Table I and Figs. 1 and 2). As one can also see in Figs. 1 and 2 and in Table I, in the high barrier limit λ_1 is in excellent agreement with λ_1^{as} , calculated from the asymptotic Eq. (29). Thus Eq. (28) may be used to calculate λ_1 for all values of σ . Figure 2 also shows the depletion effect, which consists of the drastic deviation of the relaxation time τ [Eq. (30)] from λ_1^{-1} in the low temperature limit starting from some critical values h_c of the parameter h and that is due to depletion of the upper (shallow) potential well involved into the relaxation process. The critical value is known to be $h_c \approx 0.17$ [26]. The phenomenon was discovered for uniaxial particles by Coffey *et al.* [27] and later explained by Garanin [26], who showed that this effect is a natural consequence of the depletion of the shallower of the two potential wells (which are involved in the barrier crossing) by the uniform field. Thus at low temperatures the fast modes may come to dominate the relaxation. Furthermore, in Ref. [4] it has been shown that this depletion effect always exists in relaxation in bistable potentials and it has also been asserted that such an effect is a general feature of relaxation in biased double well potentials.

IV. UNIAXIAL PARTICLES IN OBLIQUE FIELD

In general the field \mathbf{H}_0 may be applied at some angle to the easy axis of the particle. In this case, free energy per unit volume has the form

$$\begin{aligned} V &= -(\mathbf{M} \cdot \mathbf{H}_0) - K \cos^2 \theta \\ &= -H_0 M_S \sqrt{\frac{2\pi}{3}} \{ (\gamma_X + i\gamma_Y) Y_{1,-1} + \gamma_Z \sqrt{2} Y_{1,0} \\ &\quad - (\gamma_X - i\gamma_Y) Y_{1,1} \} - \frac{4K}{3} \sqrt{\frac{\pi}{5}} Y_{2,0} - \frac{K}{3}. \end{aligned} \quad (33)$$

where $\gamma_X, \gamma_Y, \gamma_Z$ are the direction cosines of the field \mathbf{H}_0 . This problem has recently been investigated in Refs. [16,29,30]. However, it has become apparent that Eq. (13) used in those papers for the numerical calculation of λ_1 were not applicable at small damping ($\alpha < 0.01$) and high barriers ($\sigma > 10$). In order to demonstrate the versatility of the matrix-continued fraction approach, we show below that it works well at those ranges of the parameters α and σ where traditional methods fail.

As has been described in detail in Refs. [14,31], the longitudinal relaxation of the particle is governed by a system of 11-term recurrence equations for the equilibrium correlation functions $c_{n,m}(t)$:

$$\tau_N \frac{d}{dt} c_{l,m}(t) = \sum_{l'=-2}^2 \sum_{s=-1}^1 d_{l+l',m\pm s,l,m} c_{l+l',m\pm s}(t), \quad (34)$$

where

$$\begin{aligned} c_{n,m}(t) &= \langle \cos \vartheta(0) Y_{n,m}(t) \rangle_0 - \langle \cos \vartheta(0) \rangle_0 \\ &\quad \times \langle \cos \vartheta(0) Y_{n,m}(t) \rangle_0. \end{aligned} \quad (35)$$

Equations for the $d_{n,m,r,s}$ are given in Refs. [14,31]. Having determined $c_{1,0}(t)$ and $c_{1,1}(t)$ from Eq. (34), one can evaluate the normalized longitudinal relaxation function of the magnetization [31]:

$$C_{\parallel}(t) = \frac{\gamma_Z c_{1,0}(t) - \sqrt{2} \operatorname{Re}\{(\gamma_X - i\gamma_Y) c_{1,1}(t)\}}{\gamma_Z c_{1,0}(0) - \sqrt{2} \operatorname{Re}\{(\gamma_X - i\gamma_Y) c_{1,1}(0)\}}.$$

The relaxation time τ of $C_{\parallel}(t)$ is then given by

$$\tau = \frac{1}{C_{\parallel}(0)} \int_0^{\infty} C_{\parallel}(t) dt. \quad (36)$$

The matrix-continued fraction solution of Eq. (34) is as follows. Let us introduce a vector $\mathbf{C}_n(t)$, consisting of 8n elements:

$$\mathbf{C}_n(t) = \begin{pmatrix} c_{2n,-2n}(t) \\ c_{2n,-2n+1}(t) \\ \vdots \\ c_{2n,2n}(t) \\ c_{2n-1,-2n+1}(t) \\ c_{2n-1,-2n+2}(t) \\ \vdots \\ c_{2n-1,2n-1}(t) \end{pmatrix}, \quad (37)$$

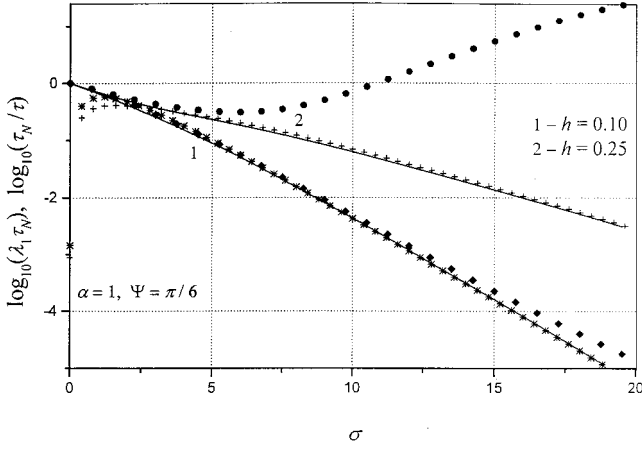


FIG. 3. λ_1 [Eq. (16)—solid lines] for the oblique field potential as a function of the barrier height σ compared with the asymptotic IHD solution λ_1^{IHD} [Eq. (39)] (stars and crosses) and the solution rendered by the inverse of the correlation time τ^{-1} [Eq. (36)] (diamonds and filled circles). Here we have taken $\gamma_X = \sin \Psi$, $\gamma_Y = 0$, $\gamma_Z = \cos \Psi$.

with $\mathbf{C}_0(t) = \mathbf{0}$. Then Eq. (34) can be transformed [31] in a matrix three-term differential-recurrence equation (1), where the matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- are described in detail in the Appendix.

In the context of the continued fraction approach, the smallest eigenvalue λ_1 is determined by Eq. (19). The results of the calculation of λ_1 from Eq. (19) are presented in Figs. 3 and 4, where they are compared with asymptotic estimates for λ_1 . The calculation of asymptotic estimates of λ_1 for the oblique field problem is well documented [16,29,30]. Here the axially symmetric asymptote for λ_1 , Eq. (29), may be used only if the field \mathbf{H}_0 is parallel to the easy axis and there is uniaxial anisotropy. In other cases, the range of values of the damping factor α , for which a particular escape rate formula is valid, must be taken into account [10] just as in the conventional Kramers theory [25] of the escape of particles over potential barriers.

In order to evaluate λ_1 in the intermediate to high damping (IHD) limit, i.e., for $\alpha \geq 1$, it is supposed [7] that the free

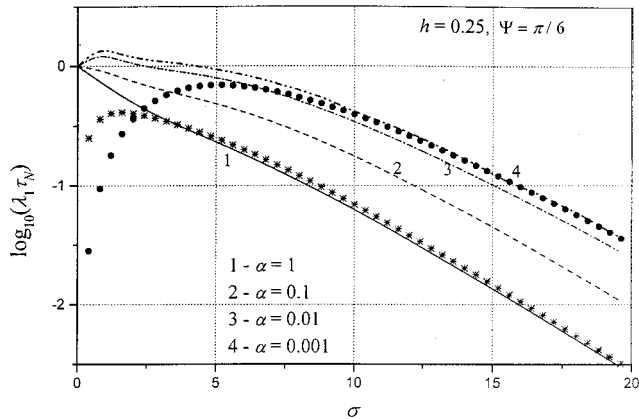


FIG. 4. λ_1 [Eq. (16)—curves 1–4] for the oblique field potential at $h = 0.25$ as a function of the barrier height σ for various values of the damping parameter α compared with the asymptotic IHD solution λ_1^{IHD} [Eq. (39)] (stars) and the asymptotic LD solution λ_1^{LD} [Eq. (42)] (filled circles).

energy per unit volume $V(\mathbf{M})$ has a bistable structure with minima at \mathbf{n}_1 and \mathbf{n}_2 separated by a potential barrier that contains a saddle point at \mathbf{n}_0 . If $(\alpha_1^{(i)}, \alpha_2^{(i)}, \alpha_3^{(i)})$ denote the direction cosines of \mathbf{M} , and \mathbf{M} is close to the stationary point \mathbf{n}_i of the potential, then $V(\mathbf{M})$ can be approximated to second order in $\alpha^{(i)}$ as

$$V = V_i + \frac{1}{2} [c_1^{(i)} (\alpha_1^{(i)})^2 + c_2^{(i)} (\alpha_2^{(i)})^2]. \quad (38)$$

Upon substituting Eq. (38) into the FPE (7), the latter may be solved in the vicinity of the saddle point to yield [7,14]

$$\lambda_1^{\text{IHD}} \sim \frac{\Omega_0}{2\pi\omega_0} \{ \omega_1 e^{-\beta(V_0 - V_1)} + \omega_2 e^{-\beta(V_0 - V_2)} \}, \quad (39)$$

where

$$\omega_1^2 = \frac{\gamma^2}{M_s^2} c_1^{(1)} c_2^{(1)}, \quad \omega_2^2 = \frac{\gamma^2}{M_s^2} c_1^{(2)} c_2^{(2)}, \quad \omega_0^2 = -\frac{\gamma^2}{M_s^2} c_1^{(0)} c_2^{(0)} \quad (40)$$

are the squares of the well and saddle angular frequencies, respectively, and the (over)damped saddle angular frequency Ω_0 is

$$\Omega_0 = \frac{h'}{2} [-c_1^{(0)} - c_2^{(0)} + \sqrt{(c_2^{(0)} - c_1^{(0)})^2 - 4\alpha^{-2} c_1^{(0)} c_2^{(0)}}]. \quad (41)$$

Equation (39) is clearly of the same form as the IHD formula derived by Kramers [25]. Equations for V_i and ω_i are given elsewhere [14].

A low damping (LD) asymptotic formula for λ_1 in the energy diffusion controlled [25] limit, i.e., for $\alpha \ll 1$, was derived by Klik and Gunther [9]. Their formula applied to the present problem yields [9,11]

$$\lambda_1^{\text{LD}} \sim \frac{\omega_1 \Delta E}{\pi k T} e^{-\beta(V_0 - V_1)}, \quad (42)$$

where ω_1 is the frequency of oscillation in the potential well 1,

$$\Delta E = \alpha \nu \oint_{V=V_0} \left[(1 - u_z^2) \frac{\partial}{\partial u_z} V d\varphi - \frac{1}{1 - u_z^2} \frac{\partial}{\partial \varphi} V du_z \right] \quad (43)$$

is the energy loss per circle of the almost periodic motion at the saddle point energy νV_0 , and $u_z = \cos \vartheta$. Here instead of the numerical evaluation of the integral in Eq. (43) (which is of the order of the barrier height [9]) we have used an approximation $\Delta E \approx \alpha \nu V_0$.

In the IHD limit, the lowest eigenvalue λ_1 from Eq. (19) is in good agreement with the asymptotic solution λ_1^{IHD} [Eq. (39)] at high σ (Fig. 3). Just as for the uniaxial problem, $h < h_c$, λ_1 and τ^{-1} are very close to each other for all barrier heights. However, for $h > h_c$ the depletion effect appears and λ_1 and τ^{-1} diverge exponentially. In Fig. 4, λ_1^{LD} calculated from the asymptotic Eq. (42) is also presented. As one can see in Fig. 4, in contrast to the biased uniaxial potential (Sec. III) λ_1 for the oblique field problem strongly depends on the damping parameter α . As one can see, λ_1 is in good agree-

ment with the asymptotic estimates for both the IHD and LD limits. Here the LD limit corresponds to values of $\alpha \leq 0.001$ that are in agreement with the independent calculation [32]. However, for crossover values of α (at about $\alpha \approx 0.05$) neither the IHD formula (39) nor the LD Eq. (42) yield reliable quantitative estimates. Here a more detailed analysis is necessary [32] in order to obtain asymptotic formulas.

V. CONCLUSIONS

We have derived an approximate formula [Eq. (19)] for the smallest nonvanishing eigenvalue λ_1 using the matrix-continued fraction approach for the problem of the Brownian motion in a potential, whose relaxation behavior is governed by multiterm recurrence relations for the moments (the expectation values of the dynamic quantities of interest). As was demonstrated on several examples, the results of this matrix-continued fraction approach are in agreement with those obtained by independent methods and, furthermore, this approach may be used to evaluate λ_1 in those ranges of parameters where traditional methods fail or their application encounters difficulties. In the IHD limit, the condition of the applicability ($\tau_e \lambda_1 \ll 1$) of Eq. (19) is valid in the high barrier (or low temperature) limit. Moreover, as we have demonstrated, Eq. (19) also provides a sufficient accuracy for intermediate and small barrier heights, where $\tau_e \lambda_1 \leq 1$. This has the merit that in the IHD limit one now has an equation for λ_1 at all ranges of the barrier heights. We have shown in Sec. IV that the continued fraction approach may be very useful in the evaluation of λ_1 in the low damping limit as well. However, in this limit the condition $\tau_e \lambda_1 \ll 1$ may be broken in some cases (e.g., for relaxation of superparamagnetic particles with cubic anisotropy for small and intermediate barriers, where $\tau_e \lambda_1 \gg 1$ [15]) and thus Eq. (19) is no longer applicable for the evaluation of λ_1 . Here, there is also a general restriction of the matrix-continued fraction approach in the calculation of λ_1 based on Eq. (12) [2], viz, for very small damping the dimension of matrices to be inverted may increase considerably and/or the matrices involved may

become badly conditioned so that the method is no longer applicable for numerical calculations (e.g., for the model considered in Sec. IV the computational problems arise at $\alpha < 10^{-4}$).

ACKNOWLEDGMENTS

I thank Professor W. T. Coffey, Professor J. L. Déjardin, Dr. P. M. Déjardin, and Dr. S. V. Titov for useful discussions. The support of this work by the International Association for the Promotion of Cooperation with Scientists from the New Independent States of the Former Soviet Union (Grant No. INTAS 96-0663) is gratefully acknowledged.

APPENDIX: THE MATRICES \mathbf{Q}_n , \mathbf{Q}_n^+ , \mathbf{Q}_n^- FOR THE OBLIQUE FIELD PROBLEM

Equation (34) can be presented in the form of Eq. (1), where the matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- are given by [31]

$$\mathbf{Q}_n = \begin{pmatrix} \mathbf{X}_{2n} & \mathbf{W}_{2n} \\ \mathbf{Y}_{2n-1} & \mathbf{X}_{2n-1} \end{pmatrix}. \quad (\text{A1})$$

$$\mathbf{Q}_n^+ = \begin{pmatrix} \mathbf{Z}_{2n} & \mathbf{Y}_{2n} \\ \mathbf{O} & \mathbf{Z}_{2n-1} \end{pmatrix}. \quad (\text{A2})$$

$$\mathbf{Q}_n^- = \begin{pmatrix} -\frac{2n+1}{2n-2} \mathbf{Z}_{2n-2}^T & \mathbf{O} \\ \mathbf{W}_{2n-1} & -\frac{2n}{2n-3} \mathbf{Z}_{2n-3}^T \end{pmatrix}, \quad (\text{A3})$$

where the superscript T in Eq. (A3) means the transposition and \mathbf{O} is the zero matrix of appropriate dimension. The dimensions of the matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- are accordingly equal to $8n \times 8n$, $8n \times 8(n+1)$, and $8n \times 8(n-1)$. The exception is \mathbf{Q}_1^- , which degenerates to a column vector of dimension 8. The submatrices \mathbf{X}_l , \mathbf{Y}_l , \mathbf{W}_l , \mathbf{Z}_l in Eqs. (A1)–(A3) are given by [31]

$$\mathbf{X}_l = \begin{pmatrix} x_{l,-l} & x_{l,-l}^+ & 0 & \cdots & 0 & 0 \\ x_{l,-l+1}^- & x_{l,-l+1} & x_{l,-l+1}^+ & \cdots & 0 & 0 \\ 0 & x_{l,-l+2}^- & x_{l,-l+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x_{l,l-1} & x_{l,l-1}^+ \\ 0 & 0 & 0 & \cdots & x_{l,l}^- & x_{l,l} \end{pmatrix},$$

$$\mathbf{Y}_l = \begin{pmatrix} y_{l,-l}^- & y_{l,-l} & y_{l,-l}^+ & \cdots & 0 & 0 & 0 \\ 0 & y_{l,-l+1}^- & y_{l,-l+1} & \cdots & 0 & 0 & 0 \\ 0 & 0 & y_{l,-l+2}^- & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & y_{l,l-1} & y_{l,l-1}^+ & 0 \\ 0 & 0 & 0 & \cdots & y_{l,l}^- & y_{l,l} & y_{l,l}^+ \end{pmatrix},$$

$$\mathbf{W}_l = \begin{pmatrix} w_{l,-l}^+ & 0 & 0 & \cdots & 0 & 0 \\ w_{l,-l+1} & w_{l,-l+1}^+ & 0 & \cdots & 0 & 0 \\ w_{l,-l+2}^- & w_{l,-l+2} & w_{l,-l+2}^+ & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & w_{l,l-2} & w_{l,l-2}^+ \\ 0 & 0 & 0 & \cdots & w_{l,l-1}^- & w_{l,l-1} \\ 0 & 0 & 0 & \cdots & 0 & w_{l,l}^- \end{pmatrix},$$

$$\mathbf{Z}_l = \begin{pmatrix} 0 & 0 & z_{l,-l} & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_{l,-l+1} & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & z_{l,l-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & z_{l,l} & 0 & 0 \end{pmatrix}.$$

The elements of \mathbf{X}_l , \mathbf{Y}_l , \mathbf{W}_l , \mathbf{Z}_l are

$$x_{l,m} = \frac{\sigma[l(l+1)-3m^2]}{(2l-1)(2l+3)} - \frac{l(l+1)}{2} - i \frac{m\sigma h \gamma_Z}{\alpha},$$

$$x_{l,m}^+ = -(x_{l,-m}^-)^* = -i \frac{\sigma h (\gamma_X - i \gamma_Y)}{2\alpha} \sqrt{(l+m+1)(l-m)},$$

$$y_{l,m} = -\sigma \left(\gamma_Z h l + i \frac{m}{\alpha} \right) \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}},$$

$$y_{l,m}^+ = -(y_{l,-m}^-)^* = \frac{l\sigma h (\gamma_X - i \gamma_Y)}{2} \sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}},$$

$$w_{l,m} = \sigma \left(h \gamma_Z (l+1) - i \frac{m}{\alpha} \right) \sqrt{\frac{l^2 - m^2}{4l^2 - 1}}.$$

$$w_{l,m}^+ = -(w_{l,-m}^-)^* = \frac{(l+1)\sigma h (\gamma_X - i \gamma_Y)}{2} \sqrt{\frac{(l-m)(l-m-1)}{4l^2 - 1}},$$

$$z_{l,m} = -\frac{\sigma l}{2l+3} \sqrt{\frac{[(l+2)^2 - m^2][(l+1)^2 - m^2]}{(2l+1)(2l+5)}}.$$

The vectors of the initial conditions $\mathbf{C}_n(0)$ appearing in Eq. (2) can also be calculated with the help of matrix-continued fractions. Namely, it can be shown [31] that the equilibrium averages $\langle Y_{n,m} \rangle_0$ satisfy the matrix recurrence relation

$$\mathbf{Q}_n^- \mathbf{R}_{n-1} + \mathbf{Q}_n \mathbf{R}_n + \mathbf{Q}_n^+ \mathbf{R}_{n+1} = \mathbf{0}, \quad n = 1, 2, 3, \dots, \quad (\text{A4})$$

where

$$\mathbf{R}_n = \begin{pmatrix} \langle Y_{2n,-2n} \rangle_0 \\ \langle Y_{2n,-2n+1} \rangle_0 \\ \vdots \\ \langle Y_{2n,2n} \rangle_0 \\ \langle Y_{2n-1,-2n+1} \rangle_0 \\ \langle Y_{2n-1,-2n+2} \rangle_0 \\ \vdots \\ \langle Y_{2n-1,2n-1} \rangle_0 \end{pmatrix},$$

and $\mathbf{0}$ is a zero column vector. The solution of Eq. (A4) is given by

$$\mathbf{R}_n = \mathbf{S}_n \mathbf{R}_{n-1} = \frac{1}{\sqrt{4\pi}} \prod_{k=1}^n \mathbf{S}_k,$$

where \mathbf{S}_n is the matrix-continued fraction defined as

$$\mathbf{S}_n = [-\mathbf{Q}_n - \mathbf{Q}_n^+ \mathbf{S}_{n+1}]^{-1} \mathbf{Q}_n^-.$$

Thus the initial conditions $\mathbf{C}_n(0)$ are given by

$$\mathbf{C}_n(0) = \frac{1}{\sqrt{4\pi}} [\hat{\mathbf{K}}_n + (\mathbf{K}_n + \hat{\mathbf{K}}_{n+1}^H \mathbf{S}_{n+1}) \mathbf{S}_n] \prod_{k=1}^{n-1} \mathbf{S}_k.$$

where

$$\mathbf{K}_n = \begin{pmatrix} \mathbf{F}_{2n} & \mathbf{D}_{2n} \\ \mathbf{D}_{2n}^H & \mathbf{F}_{2n-1} \end{pmatrix}, \quad \hat{\mathbf{K}}_n = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{2n-1} & \mathbf{0} \end{pmatrix},$$

with

$$\hat{\mathbf{K}}_1 = \begin{pmatrix} \mathbf{0} \\ \mathbf{D}_1 \end{pmatrix}$$

(the superscript H denotes the Hermitian conjugate, i.e., the transposition and the complex conjugate). The matrices \mathbf{K}_n , $\hat{\mathbf{K}}_n$ consist of two submatrices:

$$\mathbf{F}_l = -\sqrt{\frac{4\pi}{3}} \operatorname{Re}[\gamma_Z \langle Y_{1,0} \rangle_0 - \sqrt{2}(\gamma_X - i\gamma_Y) \langle Y_{1,1} \rangle_0] \mathbf{I},$$

and \mathbf{D}_l , which has the same form as the submatrix \mathbf{W}_l . The dimensions of \mathbf{F}_l and \mathbf{D}_l are equal to $(2l+1) \times (2l+1)$ and $(2l+1) \times (2l-1)$, respectively. The elements of the submatrix \mathbf{D}_l are given by

$$d_{l,m} = \gamma_Z \sqrt{\frac{l^2 - m^2}{4l^2 - 1}},$$

$$d_{l,m}^- = -(d_{l,-m}^+)^* = \frac{(\gamma_X + i\gamma_Y)}{2} \sqrt{\frac{(l+m-1)(l+m)}{4l^2 - 1}}.$$

It was verified by means of the numerical calculation that the matrices \mathbf{Q}_n , \mathbf{Q}_n^+ , and \mathbf{Q}_n^- given by Eqs. (24)–(26) fulfil the conditions (27). This guarantees the convergence of the matrix-continued fraction $\Delta_n(0)$ defined by Eq. (3).

-
- [1] Yu. P. Kalmykov, Phys. Rev. E **61**, 6320 (2000).
- [2] H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1989).
- [3] W. T. Coffey, Yu. P. Kalmykov, and J. T. Waldron, *The Langevin Equation* (World Scientific, Singapore, 1996).
- [4] W. T. Coffey, D. S. F. Crothers, and Yu. P. Kalmykov, Phys. Rev. E **55**, 4812 (1997).
- [5] C. P. Bean and J. D. Livingston, J. Appl. Phys., Suppl. **30**, 120S (1959).
- [6] W. Wernsdorfer, B. Doudin, D. Mailly, K. Hasselbach, A. Benoit, J. Meier, J.-Ph. Ansermet, and B. Barbara, Phys. Rev. Lett. **77**, 1873 (1996).
- [7] W. F. Brown, Jr., IEEE Trans. Magn. **15**, 1196 (1979).
- [8] Yu. L. Raikher and M. I. Shliomis, in *Relaxation Phenomena in Condensed Matter*, edited by W. T. Coffey, Vol. 87 of *Advances in Chemical Physics*, edited by I. Prigogine and S. A. Rice (Wiley, New York, 1994), p. 595.
- [9] I. Klik and L. Gunther, J. Stat. Phys. **60**, 473 (1990).
- [10] P. Hänggi, P. Talkner, and M. Borkovec, Rev. Mod. Phys. **62**, 251 (1990).
- [11] W. T. Coffey, in *Advances in Chemical Physics*, edited by I. Prigogine and S. A. Rice (Wiley, New York, 1998), Vol. 103, p. 259.
- [12] R. N. Zare, *Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics* (Wiley, New York, 1988).
- [13] Yu. P. Kalmykov and S. V. Titov, Phys. Rev. Lett. **82**, 2967 (1999).
- [14] L. J. Geoghegan, W. T. Coffey, and B. Mulligan, in *Advances in Chemical Physics*, edited by I. Prigogine and S. A. Rice (Wiley, New York, 1997), Vol. 100, p. 475.
- [15] Yu. P. Kalmykov, S. V. Titov, and W. T. Coffey, Phys. Rev. B **58**, 3267 (1998).
- [16] W. T. Coffey, D. S. F. Crothers, J. L. Dormann, L. J. Geoghegan, and E. C. Kennedy, Phys. Rev. B **58**, 3249 (1998).
- [17] G. A. Korn and T. M. Korn, *Mathematical Handbook* (McGraw-Hill, New York, 1968).
- [18] A. Aharoni, Phys. Rev. **177**, 763 (1969).
- [19] D. A. Garanin, V. V. Ischenko, and L. V. Panina, Teor. Mat. Fiz. **82**, 242 (1990) [Theor. Math. Phys. **82**, 169 (1990)].
- [20] Yu. L. Raikher, V. I. Stepanov, A. N. Grigorenko, and P. I. Nikitin, Phys. Rev. E **56**, 6400 (1997).
- [21] W. H. de Jeu, *Physical Properties of Liquid Crystalline Materials* (Gordon and Breach, New York, 1980).
- [22] J.-L. Déjardin, *Dynamic Kerr Effect* (World Scientific, Singapore, 1995).
- [23] L. Néel, Ann. Geophys. (C.N.R.S.) **5**, 99 (1949).
- [24] W. F. Brown, Phys. Rev. **130**, 1677 (1963).
- [25] H. A. Kramers, Physica (Amsterdam) **7**, 284 (1940).
- [26] D. A. Garanin, Phys. Rev. E **54**, 3250 (1996).
- [27] W. T. Coffey, D. S. F. Crothers, Yu. P. Kalmykov, and J. T. Waldron, Phys. Rev. B **51**, 15 947 (1995).
- [28] H. Denk and M. Riederle, J. Approx. Theory **35**, 355 (1982).
- [29] W. T. Coffey, D. S. F. Crothers, J. L. Dormann, L. J. Geoghegan, and E. C. Kennedy, Phys. Rev. B **58**, 3249 (1998).
- [30] W. T. Coffey, D. S. F. Crothers, J. L. Dormann, L. J. Geoghegan, and E. C. Kennedy, J. Phys.: Condens. Matter **10**, 3249 (1998).
- [31] Yu. P. Kalmykov and S. V. Titov, Fiz. Tverd. Tela (S.-Peterburg) **40**, 1642 (1998) [Phys. Solid State **40**, 1492 (1998)].
- [32] D. A. Garanin, E. C. Kennedy, D. S. F. Crothers, and W. T. Coffey, Phys. Rev. E **60**, 6499 (1999).