A

Continued Fraction Solutions of Eq. (5.301)

Upon defining the Fourier transforms $F_n^{(1)}(\omega) = \int_{-\infty}^{\infty} f_n^{(1)}(t) \mathrm{e}^{\mathrm{i}\omega t} \mathrm{d}t$, we have an exact solution of (5.301) (details in [143], [329])

$$\begin{aligned} F_1^{(1)}(\omega) = & \frac{\xi_\omega \left(1 - \langle P_2 \rangle_0\right)/3}{\mathrm{i}\omega\tau_D + 1 - 2\sigma[1 - S_3(\omega)]/5} \\ & \times \left[1 + \frac{2}{\sqrt{\pi}} \sum_{n=1}^{\infty} (-1)^n \frac{\Gamma(n+3/2)(f_{2n}^{(0)} - f_{2n+2}^{(0)})}{\Gamma(n+1)(1 - \langle P_2 \rangle_0)} \prod_{k=1}^{n} S_{2k+1}(\omega)\right] \end{aligned} \tag{A.1}$$

where the infinite continued fractions $S_n(\omega)$ are defined by the recurrence relation

$$S_n(\omega) = c_n[\mathrm{i}\omega\tau_D - d_n - g_n S_{n+2}(\omega)]^{-1} \tag{A.2}$$

$$f_{2n}^{(0)} = \langle P_{2n} \rangle_0 = \frac{\sigma^n \Gamma(n+1/2)}{2\Gamma(2n+3/2)} \frac{M(n+1/2, 2n+3/2, \sigma)}{M(1/2, 3/2/\sigma)}$$

$$M(a, b, z) = \frac{\Gamma(b)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n) z^n}{\Gamma(b+n) n!}$$

is the confluent hypergeometric (Kummer) function [1]. Equation (A.1) with ξ_ω omitted is, in fact, the complex susceptibility $\chi_1(\omega)$ associated with the matrix element $f_1^{(1)}(t)$, that is, the mean dipole moment. Equation (A.1) may be rewrittten as

$$\begin{aligned} F^{(1)}(0) = & \tfrac{\xi_\omega}{6} M(1, 5/2, \sigma) \Big[\tfrac{M(1/2,5/2,\sigma)}{M(1/2,3/2,\sigma)} \\ & + \textstyle\sum_{n=1}^{\infty} \tfrac{(-1)^n (2n+1)(n+1) \Gamma(n+1/2)}{\Gamma(n+2) \Gamma(1/2)} \\ & \times \tfrac{\sigma^n \Gamma(n+1/2)}{\Gamma(2n+3/2)} \tfrac{M(n+1/2,2n+5/2,\sigma)}{2M(1/2,3/2,\sigma)} \\ & \times \tfrac{n! \sigma^n}{2^{2n} (5/4)_n (7/4)_n} \tfrac{M(n+1,2n+5/2,\sigma)}{M(1,5/2,\sigma)} \Big] \end{aligned} \tag{A.3}$$

Equation (A.3) can be further simplified by absorbing the first term within the square brackets into the infinite sum. On doing this we obtain using the properties of the Pochhammer symbol specifically

$$2^{2n}(5/4)_n(7/4)_n = (5/2)_{2n}$$

$$\frac{(3/2)_n}{(3/2)_{2n}} = \frac{\Gamma(n+3/2)}{\Gamma(2n+3/2)}$$

we get

$$\begin{aligned} F^{(1)}(0) =& \frac{\xi_\omega}{6}\frac{1}{M(1/2,3/2,\sigma)}\sum_{n=0}^{\infty}\frac{(-1)^n(1/2)_n(3/2)_n\sigma^{2n}}{(3/2)_{2n}(5/2)_{2n}} \\ &\times M(n+1/2,2n+5/2,\sigma)M(n+1,2n+5/2,\sigma) \end{aligned} \tag{A.4}$$

Equation (A.4) is still of reasonably complicated mathematical form as it involves infinite summations of products of infinite summations. This difficulty may be overcome by noting that from [499] vol. 3 (6.6.2) part 9:

$$\begin{aligned} &\sum_{k=0}^{\infty}(-1)^k\frac{(a)_k(a')_k(b-1)_k}{k!(b-1)_{2k}(b)_{2k}}x^ky^kM(a+k,b+2k,x)M(a'+k,b+2k,y) \\ &= \Phi_2(a,a';b;x,y) \end{aligned} \tag{A.5}$$

This is proven from first principles by changing the order of summations. Thus on making the substitutions

$$k=n\,,\quad x=y=\sigma\,,\quad a=1/2\,,\quad a'=1\,,\quad b=5/2 \tag{A.6}$$

$$\begin{aligned} &\sum_{n=0}^{\infty}(-1)^n\frac{(1/2)_n(1)_n(3/2)_n\sigma^{2n}}{n!(3/2)_{2n}(5/2)_{2n}}M\left(\frac{1}{2}+n,\frac{5}{2}+2n,\sigma\right) \\ &\qquad\times M\left(1+n,\frac{5}{2}+2n,\sigma\right) = \Phi_2\left(\frac{1}{2},1;\frac{5}{2};\sigma,\sigma\right) \end{aligned}$$

so that the summation disappears and we have the simple relation

$$F_1^{(1)}(0) = \frac{\xi_\omega}{6M(1/2,3/2,\sigma_0)}\Phi_2\left(1,\frac{1}{2};\frac{5}{2};\sigma,\sigma\right) \tag{A.7}$$

where Φ_2 is the degenerate Appell function given by

$$\begin{aligned} \Phi_2(b,b';c;w,z) =& \frac{\Gamma(c)}{\Gamma(b)\Gamma(b')\Gamma(c-b-b')} \\ &\iint u^{b-1}v^{b'-1}(1-u-v)^{c-b-b'-1}\mathrm{e}^{uw+vz}\mathrm{d}u\mathrm{d}v \end{aligned} \tag{A.8}$$

where the double integral is performed subject to u, $v \geq 0$ and $u+v \leq 1$. Here it is assumed ([499], vol 3 p 451 (49)) that $\mathrm{Re}\{\mathrm{b},\mathrm{b}',\mathrm{c}-\mathrm{b}-\mathrm{b}'\} > 0$. Accordingly the Φ_2 in (A.7) may be evaluated as a repeated integral given by

$$\frac{3}{4}\int_0^1 \mathrm{d}v\, v^{-1/2}\exp(\sigma v)\int_0^{1-v}\mathrm{d}u\exp(\sigma u) \tag{A.9}$$

$$= \frac{3}{4\sigma_0}\int_0^1 \mathrm{d}v\, v^{-1/2}[\exp(\sigma)-\exp(\sigma v)] \tag{A.10}$$

$$= \frac{3}{2\sigma_0}\int_0^1 \mathrm{d}x[\exp(\sigma)-\exp(\sigma x^2)]\ , \qquad (v = x^2) \tag{A.11}$$

$$= \frac{3}{2\sigma_0}[\exp(\sigma) - M(1/2, 3/2, \sigma)] \tag{A.12}$$

$$= \frac{3}{2\sigma}\left[\mathrm{e}^{\sigma} - \frac{\sqrt{\pi}}{2\sqrt{\sigma}} erfi(\sqrt{\sigma})\right] \tag{A.13}$$

$$= M(3/2, 5/2, \sigma) \tag{A.14}$$

where we have used (11) and (29) on pages 580–1 of Prudnikov et al., vol. 3 [499]. Thus (A.4) is reduced to the ratio of two hypergeometric functions

$$F_1^{(1)}(0) = \frac{\xi_\omega M(3/2, 5/2, \sigma)}{6M(1/2, 3/2, \sigma)} \tag{A.15}$$

and [130] the static susceptibility is given by

$$\chi(0) = 2\mu F_1^{(1)}(0) = \frac{\mu\xi_\omega}{3\sigma}\left[\frac{2\sqrt{\sigma}}{\pi}\mathrm{e}^{\sigma}\{erfi(\sqrt{\sigma})\}^{-1} - 1\right] \tag{A.16}$$

This agrees, as it should, with the equation after equation (33) of [130], which is the static susceptibility as rendered by the equilibrium distribution, upon identifying the constants

$$\mu\xi_\omega = \frac{m^2 N}{kT} \tag{A.17}$$

We remark, by linear response theory, that the matrix elements $f_{2n-1}^{(1)}(t)$ may also be expressed [558] in terms of the equilibrium correlation functions

$$\Phi_{1,2n-1}(t) = \langle\cos\vartheta(0)P_{2n-1}[\cos\vartheta(t)]\rangle_0 / \langle\cos\vartheta(0)P_{2n-1}[\cos\vartheta(0)]\rangle_0$$

as

$$f_{2n-1}^{(1)}(t) = -\chi_{2n-1}\int_{-\infty}^{t}\dot{\Phi}_{1,2n-1}(t-t')\xi(t')\mathrm{d}t' \tag{A.18}$$

where $\chi_{2n-1} = \langle\cos\vartheta(0)P_{2n-1}[\cos\vartheta(0)]\rangle_0$. This is a useful representation of the solution as, in general, it is much easier to calculate $\Phi_{1,2n-1}(t)$, the after-effect solution rather than the ac response directly. The corresponding hierarchy of linear complex susceptibilities is

$$\chi_{2n-1}(\omega) = \chi_{2n-1}\left[1 - \mathrm{i}\omega\int_0^{\infty}\Phi_{1,2n-1}(t)\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}t\right]$$

so that in (5.293) $\chi(\omega)$ corresponds to $\chi_1(\omega)$.

It may also be shown by continued-fraction methods suitably adopted, how the matrix element $f_2^{(2)}(t)$ for a pure ω sinusoid $\xi(t) = \xi_m \cos \omega_0 t$ may be given (details in [143], [329], Appendix C)

$$f_2^{2)}(t) = \mathrm{Re}\left\{\mathrm{F}_0^{(2)}(\omega_0) + \mathrm{F}_2^{(2)}(2\omega_0)\mathrm{e}^{2\mathrm{i}\omega_0 \mathrm{t}}\right\} \tag{A.19}$$

where

$$\begin{pmatrix} F_0^{(2)}(\omega_0) \\ F_2^{(2)}(2\omega_0) \end{pmatrix} = \frac{3\sqrt{\pi}\xi_m^2}{8\sigma} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}\Gamma(n+1)}{\Gamma(n+1/2)} \prod_{k=1}^{n} \begin{pmatrix} S_{2k}(0) \\ S_{2k}(2\omega_0) \end{pmatrix} \times [\chi_{2n-1}(\omega_0) - \chi_{2n+1}(\omega_0)] \tag{A.20}$$

and the continued fractions S_n are again defined by (A.2).

B

Mittag–Leffler Functions

B.0.1 Properties of Mittag–Leffler Functions

$$\begin{aligned} E_{\alpha,\beta}(z) &= \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{(0+)} \frac{t^{\alpha-\beta} \mathrm{e}^{t}}{t^{\alpha} - z} \mathrm{d}t && \text{(B.1)} \\ &= \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{(0+)} \mathrm{d}t \, t^{-\beta} \mathrm{e}^{t} \sum_{n=0}^{\infty} z^{n} t^{-\alpha n} && \text{(B.2)} \\ &= \sum_{n=0}^{\infty} \frac{z^{n}}{\Gamma(\beta + \alpha n)} \qquad \text{(Hankel)} \qquad \text{(small } |z|\text{)} && \text{(B.3)} \end{aligned}$$

Also, we have

$$\begin{aligned} E_{\alpha,\beta}(z) &= \left(-\frac{1}{z}\right) \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{(0+)} \mathrm{d}t \, \mathrm{e}^{t} \sum_{n=0}^{\infty} \frac{t^{\alpha-\beta+\alpha n}}{z^{n}} && \text{(B.4)} \\ &= -\frac{1}{z} \sum_{n=0}^{\infty} \frac{z^{-n}}{\Gamma(\beta - \alpha - \alpha n)} \qquad \text{(Hankel)} && \text{(B.5)} \\ &= -\frac{1}{z} E_{-\alpha,\beta-\alpha}(1/z) \qquad \text{(large } |z|\text{)} && \text{(B.6)} \end{aligned}$$

By the ratio test, in general (B.3) converges and (B.6) diverges ($0 < \alpha < 1$).

B.0.2 Asymptotics of Mittag–Leffler functions

$$\begin{aligned}
E_\alpha(z) &= \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+\alpha n)} && \text{(B.7)}\\
&= \sum_{n=0}^{\infty} \frac{z^n}{\alpha n \Gamma(\alpha n)} && \text{(B.8)}\\
&= \sum_{n=0}^{\infty} \frac{z^n}{\alpha n} \sum_{l=1}^{\infty} c_l (\alpha n)^l \qquad ([1]\ (6.1.34))(\text{NB } c = 1) && \text{(B.9)}\\
&= 1 + \sum_{L=0}^{\infty} c_{L+1}\alpha^L \sum_{n=0}^{\infty} z^n n^L \qquad (l = L+1) && \text{(B.10)}\\
&= 1 + \sum_{L=0}^{\infty} c_{L+1}\alpha^L \sum_{n=0}^{\infty} z^{n+1} (n+1)^L \qquad (n \to n+1) && \text{(B.11)}\\
&= 1 + \frac{z c_1}{1-z} + z \sum_{L=1}^{\infty} c_{L+1}\alpha^L \sum_{n=0}^{\infty} z^n (n+1)^L && \text{(B.12)}
\end{aligned}$$

where

$$\begin{aligned}
\sum_{n=0}^{\infty} z^{n+1}(n+1)^L &= \frac{1}{z}\sum_{n=0}^{\infty} (n+1)^L z^{n+1} && \text{(B.13)}\\
&= \frac{1}{z}\sum_{n=0}^{\infty} \left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^L z^{n+1} && \text{(B.14)}\\
&= \frac{1}{z}\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^L \left(\frac{z}{1-z}\right) && \text{(B.15)}\\
&= -\frac{1}{z}\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^L \frac{1}{z-1} \qquad (L \geq 1) && \text{(B.16)}\\
&= -\frac{1}{z}\frac{\mathrm{d}^L}{\mathrm{d}t^L} f(g(t)) && \text{(B.17)}
\end{aligned}$$

where we have

$$z = \mathrm{e}^t\ ,\ \ln z = t\ ,\ g(t) = \mathrm{e}^t - 1 \tag{B.18}$$

and

$$f(g(t)) = \frac{1}{g(t)} = -\frac{1}{z}\sum_{m=0}^{L} f^{(m)}(g(t)) \sum (L; a_1 - a_L)' \prod_{j=1}^{L} \{g^{(j)}(t)\}^{a_j} \tag{B.19}$$

using Faá di Bruno's formula ([1], p. 823) and summing over (see also [465])

$$\begin{aligned}
a_1 + 2a_2 + \cdots + La_L &= L && \text{(B.20)}\\
a_1 + a_2 + \cdots + a_L &= m && \text{(B.21)}
\end{aligned}$$

and where

$$\sum(L; a_1 - a_L)' \equiv S_L^{(m)} \tag{B.22}$$

namely a Stirling number of the second kind.

However,

$$g^{(j)}(t) = \mathrm{e}^t = z \qquad (1 \leq j \leq L) \tag{B.23}$$

$$\rightarrow \quad \prod_{j=1}^{L} \{g^{(j)}(t)\}^{a_j} = \mathrm{e}^{t(a_1+a_2+\cdots+a_L)} = \mathrm{e}^{mt} = z^m \tag{B.24}$$

$$\therefore \quad \sum_{n=0}^{\infty} z^n (n+1)^L = -\sum_{m=0}^{L} \frac{(-1)^m m!}{(z-1)^{m+1}} S_L^{(m)} z^m \tag{B.25}$$

since

$$f^{(m)}(g(t)) = \frac{(-1)^m m!}{\{g(t)\}^{m+1}} \tag{B.26}$$

$$\therefore \quad E_\alpha(z) = 1 + \frac{zc_1}{1-z} + \frac{1}{z} \sum_{L=1}^{\infty} c_{L+1} \alpha^L \sum_{m=0}^{L} m! \left(\frac{z}{1-z}\right)^{m+1} S_L^{(m)} \tag{B.27}$$

However

$$\sum_{m=0}^{L} (-1)^{L-m} m! S_L^{(m)} \ = \ 1 \qquad ([1]\ p.825\ IIB) \tag{B.28}$$

$$\therefore \quad E_\alpha(z) \underset{z\to\infty}{\cong} 1 + \frac{z}{1-z} \frac{-1}{z} \sum_{L=1}^{\infty} c_{L+1} (-\alpha)^L \tag{B.29}$$

$$= 1 + \frac{z}{1-z} + \frac{1}{z} + \frac{1}{\alpha z} \sum_{l=1}^{\infty} c_l (-\alpha)^l l \ (L = l-1) \tag{B.30}$$

$$= \frac{1}{1-z} + \frac{1}{z} + \frac{1}{\alpha z} \frac{1}{\Gamma(-\alpha)} \tag{B.31}$$

$$\cong -\frac{1}{z^2} - \frac{1}{z\Gamma(1-\alpha)} \cong \frac{-1}{z\Gamma(1-\alpha)} \tag{B.32}$$

Similarly, we have

$$E_{\alpha,\beta}(z)\ z \overset{\cong}{\rightarrow} \infty - \frac{1}{z\Gamma(\beta-\alpha)} \tag{B.33}$$

B.1 Check on Norm of $x^2(\tau)$

Check on equation (3.12) of [30], with

$$z = -\gamma t^\alpha \tag{B.34}$$

$$\langle x^2(\tau)\rangle = \frac{2kT}{m}\int_0^{\tau} \mathrm{d}t(\tau - t)E_\alpha(z) \tag{B.35}$$

$$= \frac{2kT}{m}\int_0^{\tau} \mathrm{d}t(\tau - t)\sum_{n=0}^{\infty}\frac{(-\gamma t^\alpha)^n}{\Gamma(1+\alpha n)} \tag{B.36}$$

$$= \frac{2kT}{m}\sum_{n=0}^{\infty}\frac{1}{\Gamma(1+\alpha n)}\times\left[\tau\frac{(-\gamma)^n t^{\alpha n+1}}{1+\alpha n} - \frac{(-\gamma)^n t^{\alpha n+2}}{2+\alpha n}\right]_{t=0}^{\tau} \tag{B.37}$$

$$= \frac{2kT}{m}\sum_{n=0}^{\infty}\frac{1}{\Gamma(1+\alpha n)}\times\left[\frac{\tau^{\alpha n+2}(-\gamma)^n}{1+\alpha n} - \frac{\tau^{\alpha n+2}(-\gamma)^n}{2+\alpha n}\right] \tag{B.38}$$

$$= \frac{2kT}{m}\sum_{n=0}^{\infty}\left[\frac{\tau^2(-\gamma\tau^\alpha)^n}{\Gamma(2+\alpha n)} - \frac{\tau^2(-\gamma\tau^\alpha)^n(1+\alpha n)}{\Gamma(3+\alpha n)}\right] \tag{B.39}$$

$$= \frac{2kT}{m}\sum_{n=0}^{\infty}\tau^2\frac{(-\gamma\tau^\alpha)^n[2+\alpha/n-1-\alpha/n]}{\Gamma(3+\alpha n)} \tag{B.40}$$

$$= \frac{2kT}{m}\tau^2 E_{\alpha,3}(-\gamma\tau^\alpha) \tag{B.41}$$

C

Nonlinear Response to Alternating Fields

A system in thermal equilibrium at temperature T disturbed by an external stimulus evolves to a new equilibrium (stationary) state. Moreover, if the energy stimulus is much lower than the thermal energy k_BT, *linear* in the stimulus) deviations of the expectation value of the relevant dynamical variable in the stationary state are sufficient to evaluate the generalized susceptibility (linear ac response) using appropriate equilibrium (stationary) correlation functions. The calculation of the nonlinear stationary (ac) response even for systems of noninteracting particles with a single coordinate is, however, much more difficult because no connection between the transient and the ac responses exists. If interactions are included the difficulties are compounded. Nonlinear dielectric relaxation and the dynamic Kerr effect of permanent dipoles in a mean field potential are naturally occurring examples.

In this context we remark that the orientational electric polarization of noninteracting permanent dipoles in an ac field $\mathbf{E}(t)$ treated by Debye [206] depends in the linear approximation in $\mathbf{E}(t)$ on the average over orientations of the Legendre polynomial $\langle P_1(\cos\vartheta)\rangle(t)$, ϑ being the polar angle of the electric dipole moment vector $\boldsymbol{\mu}$. Similar remarks apply to the magnetization of blocked noninteracting ferrofluid particles with magnetic dipole moment $\boldsymbol{\mu}$ in ac magnetic fields $\mathbf{H}(t)$ [504]. Subsequently [142]–[504] Debye's calculation was generalized to nonlinear responses. We mention $\langle P_2\rangle(t)$ governing the Kerr effect response (KER) [212]–[122] and the nonlinear dielectric effect (NLDE) [142], [567] amending $\langle P_1\rangle(t)$ to $O(E^3)$. The conclusions are [to $O(E^2)$] for the KER for a pure sinusoid that the square law nonlinearity rectifies $\mathbf{E}(t)$, yielding a frequency-dependent dc response superimposed on which is the dephased second harmonic [65]. In the NLDE, additional terms in the fundamental and in the third harmonic appear in $\langle P_1\rangle(t)$. Experimental confirmation has been reported [567], [288]. The Debye theory may not be used for dense anisotropic dipolar systems, where intermolecular interactions occur, such as nematic liquid crystals. Here dielectric relaxation is usually interpreted using as a model the noninertial rotational Brownian motion of a rodlike particle in an external potential V (e.g., [142],[403], [460], [572]). This model was used in [132], where the exact linear ac response is calculated in terms of continued fractions (using linear response theory [373]) for the Maier–Saupe uniaxial anisotropy potential:

$$V = -K\cos^2\vartheta \tag{C.1}$$

where K is the anisotropy constant. Exact solutions for the nonlinear ac response in a uniaxial potential can also be obtained by matrix continued fractions without using perturbation theory [212], [142]. However, that approach cannot yield simple formulae for experimental comparison, and it cannot provide an exact evolution equation for the ac responses for perturbation purposes. Preliminary steps towards this were made in [504], [142], [501], [503], [91] for dielectric relaxation of dipolar systems and for magnetic relaxation (super-paramagnetism) of fine single-domain ferromagnetic particles (in most respects a replica of dielectric relaxation of nematics). Here we demonstrate how by calculating from perturbation theory the linear ac response in the presence of $\mathbf{E}(t)$ one may generate the KER and all higher-order nonlinear responses. The linear response comprising an infinity of relaxation modes may be accurately represented by two modes, that of low frequency arising from the slow barrier crossing of dipoles and that of high frequency representing the infinity of fast near-degenerate "intrawell" modes approximated as a single high-frequency mode. The analytical responses are obtained, utilizing the two-mode approximation for linear response combined with Morita's treatment [438] of nonlinear response, showing how the distribution function induced by a strong perturbing field may be calculated from the Green functions in the absence of the perturbation, with linear response theory as a special case.

The cornerstone of our calculation is the Smoluchowski (Fokker–Planck) equation for the density $W(\boldsymbol{\mu}, t)$ of orientations of dipoles $\boldsymbol{\mu}$ on the surface of the unit sphere [206], [437], [142]

$$\dot{W} = [L_{FP} + L_{ext}(t)]W \tag{C.2}$$

where $L_{FP}W = (2\tau_D)^{-1}[\Delta W + \beta\nabla\cdot(W\nabla V)]$ is the unperturbed Fokker—Planck operator while $L_{\mathrm{ext}}W = (2\tau_D)^{-1}\beta\nabla\cdot(W\nabla V_{\mathrm{ext}})$ is the Zeeman energy $V_{\mathrm{ext}}W = -(\mathbf{E}\cdot\boldsymbol{\mu})$ contribution, and ∇ and Δ are the gradient and Laplacian on the surface of the unit sphere. Here $\beta = (k_BT)^{-1}$, $\tau_D = \beta\zeta/2$ is the Debye relaxation time for free diffusion, and ζ is the viscous drag coefficient. Expanding W in the $\{P_n\}$ yields [437], [142]

$$\tau_D\dot{f}_n(t) + c_nf_{n-2}(t) + d_nf_n(t) + g_nf_{n+2}(t) = \xi(t)a_n[f_{n-1}(t) - f_{n+1}(t)] \tag{C.3}$$

where $f_n(t) = \langle P_n(\cos\vartheta)\rangle(t)$ and $\xi(t) = \beta\mu E(t)$, and all the coefficients are given, e.g., in [437], [142]. One may write

$$f_n(t) = f_n^{(0)} + f_n^{(1)}(t) + f_n^{(2)}(t) + f_n^{(3)}(t) + \cdots$$

[with the superscripts denoting the relevant order in $\mathbf{E}(t)$] so that

$$\begin{aligned}\tau_D\dot{f}_n^{(m)}(t) + c_nf_{n-2}^{(m)}(t) + d_nf_n^{(m)}(t) + g_nf_{n+2}^{(m)}(t)\\ =\xi(t)a_n[f_{n-1}^{(m-1)}(t) - f_{n+1}^{(m-1)}(t)]\end{aligned} \tag{C.4}$$

Thus to calculate the matrix element $f_2^{(2)}(t)$, i.e., the lowest-order approximation to the KER, we first determine $\{f_{2n-1}^{(1)}(t)\}$ satisfying (C.4) with $m = 1$. The *exact* solutions of (C.4) for $f_{2n-1}^{(1)}(t)$ for the stationary response to $\xi(t) = \xi e^{i\omega t}$ are given by continued fractions [212]. However, in order to obtain analytical approximations, we use another method. Suppose that a small probing field $\xi_1 = \beta\mu E_1 \ll 1$ applied along the polar axis at $t = -\infty$ is removed at $t = 0$. The step off $[\xi(t) = 0$ for $t > 0]$ solution of (C.4) for $m = 1$ $f^{(1)}_{2n-1,off}(t)$, is

$$f^{(1)}_{2n-1,off}(t) = \xi_1 \chi_{2n-1} \Phi_{1,2n-1}(t) \tag{C.5}$$

where $\Phi_{1,2n-1}(t)$ are the normalized equilibrium correlation functions defined as

$$\Phi_{k,m}(t) = \frac{\langle P_k[\cos\vartheta(0)]P_m[\cos\vartheta(t)\rangle_0 - \langle P_k\rangle_0\langle P_m\rangle_0}{\langle P_k P_m\rangle_0 - \langle P_k\rangle_0\langle P_m\rangle_0} \tag{C.6}$$

$\langle P_n\rangle_0 = \langle P_n[\cos\vartheta(0)]\rangle_0$, and $\chi_{2n-1} = \langle P_1 P_{2n-1}\rangle_0$ are the static susceptibilities, which can be expressed as hypergeometric functions [132]. The Green functions $G_{2n-1}(t)$ of the unperturbed $[\xi(t) = 0]$ (C.4) with $m = 1$ is $G_{2n-1}(t) = -\dot{\Phi}_{1,2n-1}(t)$ [373]. Thus

$$f^{(1)}_{2n-1}(t) = -\chi_{2n-1} \int_{-\infty}^{t} \dot{\Phi}_{1,2n-1}(t - t')\xi(t')\mathrm{d}t' \tag{C.7}$$

If $\xi(t) = \xi \mathrm{e}^{\mathrm{i}\omega t}$, (C.7) yields $f^{(1)}_{2n-1}(t) = \chi_{2n-1}(\omega)\xi\mathrm{e}^{\mathrm{i}\omega t}$, where $\chi_{2n-1}(\omega)$ are the generalized complex susceptibilities

$$\frac{\chi_{2n-1}(\omega)}{\chi_{2n-1}} = 1 - \mathrm{i}\omega \int_0^\infty \Phi_{1,2n-1}(t)\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}t \tag{C.8}$$

The time domain behavior of $\Phi_{1,2n-1}(t)$ is characterized by the integral and effective relaxation times

$$\tau_{2n-1} = \int_0^\infty \Phi_{1,2n-1}(t)\mathrm{d}t\,, \qquad \tau^{eff}_{2n-1} = -1/\dot{\Phi}_{1,2n-1}(0) \tag{C.9}$$

Here τ^{eff}_{2n-1} is evaluated from (C.4) with $\xi(t) = 0$ using equilibrium averages as

$$\begin{aligned}\frac{\tau^{eff}_{2n-1}}{\tau_D} &= -\frac{f^{(1)}_{2n-1,off}(0)}{\tau_D \dot{f}^{(1)}_{2n-1,off}(0)} \\ &= \left\{d_{2n-1} + c_{2n-1}\frac{\langle P_1 P_{2n-3}\rangle_0}{\langle P_1 P_{2n-1}\rangle_0} + g_{2n-1}\frac{\langle P_1 P_{2n+1}\rangle_0}{\langle P_1 P_{2n-1}\rangle_0}\right\}^{-1}\end{aligned}$$

and τ_{2n-1} is given by the mean first passage time approach of Szabo [577], which for the present problem yields

$$\begin{aligned}\tau_{2n-1} = {} & \frac{2\tau_D}{Z\langle P_1 P_{2n-1}\rangle_0} \int_{-1}^{1} \mathrm{d}z \frac{\mathrm{e}^{-\sigma z^2}}{1 - z^2} \int_{-1}^{z} x\mathrm{e}^{\sigma x^2}\mathrm{d}x \\ & \times \int_{-1}^{z} P_{2n-1}(y)\mathrm{e}^{\sigma y^2}\mathrm{d}y\end{aligned}$$

where $Z = \int_{-1}^{1} \mathrm{e}^{\sigma z^2}\mathrm{d}z$ is the partition function and $\sigma = \beta K$ is the barrier height parameter. $\Phi_{1,2n-1}(t)$ may also be written as an eigensolution using the eigenvalues

$\{\xi_k\}$ of L_{FP}, viz., $\Phi_{1,2n-1}(t) = \sum_k c_k^n \mathrm{e}^{-t\lambda_k}$, where $\sum_k c_k^n = 1$ and λ_1 (essentially the Kramers escape rate) is associated with the slowest relaxation mode and so with the long-time behavior of $\Phi_{1,2n-1}(t)$; the other λ_k characterize high-frequency intrawell modes. By (C.9) $\tau_{2n-1} = \sum_k c_k^n/\lambda_k$ and $\tau_{2n-1}^{eff} = 1/\sum_k c_k^n \lambda_k$. The behavior of λ_1, τ_{2n-1}, and τ_{2n-1}^{eff} is given, for $\sigma \le 1$, by

$$\lambda_1 \tau_D = 1 - \frac{2}{5}\sigma + \cdots$$

$$\frac{\tau_{2n-1}}{\tau_D} = \frac{n! - (1/2)_n}{n(1/2)_n} + \sigma \frac{2 + 8n!/(3/2)_{n-2}}{3n(4n+1)} + \cdots$$

$$\frac{\tau_{2n-1}^{eff}}{\tau_D} = \frac{1}{n} + \frac{2\sigma}{4n^2 + n} + \cdots$$

$[(a)_n$ is the Pochhammer symbol] and, for $\sigma \gg 1$, by

$$\lambda_1 \tau_D \sim \frac{2\sigma^{3/2}\mathrm{e}^{-\sigma}}{\sqrt{\pi}} \left(1 - \frac{1}{\sigma} - \frac{3}{4\sigma^2} + \cdots\right)$$

$$\frac{\tau_{2n-1}}{\tau_D} \sim \frac{\sqrt{\pi}\mathrm{e}^{\sigma}}{2\sigma^{3/2}} \left(1 + \frac{1}{\sigma} - \frac{7 + n - 2n^2}{4\sigma^2} + \cdots\right)$$

$$\frac{\tau_{2n-1}^{eff}}{\tau_D} \sim \frac{2\sigma}{2n^2 - n} \left(1 - \frac{3}{2\sigma} + \cdots\right)$$

The spectra of $\chi_{2n-1}(\omega)$ can be accurately described at all frequencies (see Fig. C.1) by a sum of two Lorentzians, viz.,

$$\frac{\chi_{2n-1}(\omega)}{\chi_{2n-1}} = \frac{\Delta_{2n-1}}{1 + \mathrm{i}\omega/\lambda_1} + \frac{1 - \Delta_{2n-1}}{1 + \mathrm{i}\omega\tau_W^{2n-1}} \tag{C.10}$$

where Δ_{2n-1} and τ_{2n-1}^W are determineds to ensure the correct low- and high-frequency behavior of $\chi_{2n-1}(\omega)$, viz., $\chi_{2n-1}(\omega)/\chi_{2n-1} \approx 1 - \mathrm{i}\omega\tau_{2n-1}$ as $\omega \to 0$ and $\chi_{2n-1}/\chi_{2n-1}(\omega) \sim \mathrm{i}\omega\tau_{2n-1}^{eff}$ as $\omega \to \infty$, and are given by

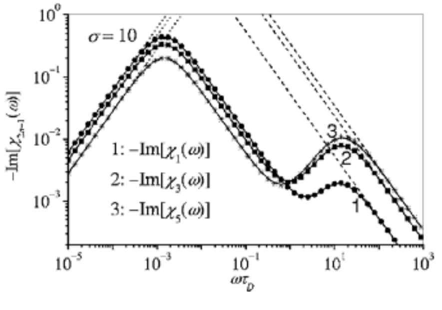

Fig. C.1. $-\mathrm{Im}\,[\chi_{2n-1}(\omega)]$ vs $\omega\tau_D$ (*solid lines*, (C.4) and (C.8) for $n = 1, 3, 5$); $\chi_{2n-1}\omega\tau_{2n-1}$ (*dotted lines*); $\chi_{2n-1}(\omega\tau_{2n-1}^{eff})^{-1}$ (*dashed lines*); symbols (C.10)

$$\varDelta_m = \frac{\tau_m/\tau_m^{eff} - 1}{\lambda_1\tau_m - 2 + 1/(\lambda_1\tau_m^{eff})}, \qquad \tau_W^m = \frac{\lambda_1\tau_m - 1}{\lambda_1 - 1/\tau_m^{eff}} \tag{C.11}$$

In the time domain, the two-mode approximation (C.10) is equivalent to assuming that the relaxation function $\varPhi_{1,2n-1}(t)$ (which in general comprises an *infinite number* of exponentials) may be approximated by *two* exponentials only. An interested reader can find a detailed description and various applications of this two-mode approximation in [142].

The second order response $\{f_{2n}^{(2)}(t)\}$ satisfies (C.4) with $m = 2$. The *exact* solution for the element $f_2^{(2)}(t)$ governing the KER, with $\xi(t) = \xi\cos\omega t$, is

$$f_2^{(2)}(t) = \xi^2 \mathrm{Re}[\mathrm{F}_0^{(2)}(\omega) + \mathrm{F}_2^{(2)}(\omega)\mathrm{e}^{2\mathrm{i}\omega\mathrm{t}}] \tag{C.12}$$

where the frequency-dependent dc $F_0^{(2)}(\omega)$ and the second harmonic $F_2^{(2)}(\omega)$ terms are

$$\begin{pmatrix} F_0^{(2)}(\omega) \\ F_2^{(2)}(\omega) \end{pmatrix} = \frac{3\sqrt{\pi}}{4\sigma}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}n!}{\varGamma(n+1/2)}\prod_{k=1}^{n}\begin{pmatrix} S_{2k}(0) \\ S_{2k}(2\mathrm{i}\omega) \end{pmatrix} \times [\chi_{2n-1}(\omega) - \chi_{2n+1}(\omega)] \tag{C.13}$$

and the continued fractions $S_n(\mathrm{i}\omega)$ are defined as $S_n(\mathrm{i}\omega) = c_n[\mathrm{i}\omega\tau_D - d_n - g_n S_{n+2}(\mathrm{i}\omega)]^{-1}$ [cf. [132], eq. (26)]. In order to obtain a simple analytic approximation for the KER, we notice that the normalized step-off solution of (C.4) with $m = 2$ is $f_{2,off}^{(2)}(t) = \xi^2\chi_2\varPhi_{2,2}(t)$, where $\varPhi_{2,2}(t)$ is the normalized second-rank equilibrium correlation function defined by (C.6) and $\chi_2 = (\langle P_2^2\rangle_0 - \langle P_2\rangle_0^2)/3$. As the overbarrier relaxation mode is not involved in the propagator of $f_2^{(2)}(t)$, one may use a single-mode approximation for $\varPhi_{2,2}(t)$, viz.,

$$\varPhi_{2,2}(t) \approx \mathrm{e}^{-t/\tau_2^{eff}} \tag{C.14}$$

with the effective relaxation time τ_2^{eff} given by

$$\frac{\tau_2^{eff}}{\tau_D} = -\frac{f_{2,off}^{(2)}(0)}{\tau_D\dot{f}_{2,off}^{(2)}(0)} = \frac{\langle P_2^2\rangle_0 - \langle P_2\rangle_0^2}{1 + \langle P_2\rangle_0 - 2\langle P_2^2\rangle_0}$$

The qualitative behavior of τ_2^{eff} is $\tau_2^{eff}/\tau_D = 1/3 + 2\sigma/189 + \cdots$ for $\sigma \leq 1$ and $\tau_2^{eff}/\tau_D = \sigma^{-1}/2 + \sigma^{-2}5/4 + \cdots$ for $\sigma \gg 1$. Moreover, using the effective relaxation time means that (C.4) for $m = 2$ can be represented as

$$\tau_2^{eff}\dot{f}_2^{(2)}(t) + f_2^{(2)}(t) = -\chi_2\xi(t)\int_{-\infty}^{t}\dot{\varPhi}^{(1)}(t-t')\xi(t')\mathrm{d}t'$$

with solution

$$f_2^{(2)}(t) = -\frac{\chi_2}{\tau_2^{eff}}\int_{-\infty}^{t}\xi(t')\mathrm{e}^{-(t-t')/\tau_2^{eff}}\int_{-\infty}^{t'}\dot{\varPhi}^{(1)}(t'-t'')\xi(t'')\mathrm{d}t''\mathrm{d}t' \tag{C.15}$$

Here $\Phi^{(1)}(t)$ is the normalized $[\Phi^{(1)}(0) = 1]$ effective relaxation function, accounting for the driving functions $\{f_{2n-1}^{(1)}(t)\}$. As before, $\Phi^{(1)}(t)$ is characterized by the integral, τ, and effective, τ^{eff}, relaxation times, which can be estimated from the low- and high-frequency asymptotes of the dc KER $\tau = -\lim_{\omega\to 0} 2\,\mathrm{Im}\,[\mathrm{F}_0^{(2)}(\omega)]/(\omega\chi_2)$ and $\tau^{eff} = -\lim_{\omega\to\infty} \chi_2\{2\omega\,\mathrm{Im}\,[\mathrm{F}_0^{(2)}(\omega)]\}^{-1}$. The one-sided Fourier transform of $-\dot{\Phi}^{(1)}(t)$ may be represented in a two-mode approximation as

$$1 - \mathrm{i}\omega\tilde{\Phi}^{(1)} = \frac{\Delta_2}{1 + \mathrm{i}\omega/\lambda_1} + \frac{1 - \Delta_2}{1 + \mathrm{i}\omega\tau_W^2} \tag{C.16}$$

Here Δ_2 and τ_W^2 may be evaluated from (C.11) using λ_1, $\tau_m = \tau$, and $\tau_m^{eff} = \tau^{eff}$ (see Table C.1). For $\sigma < 1$ and $\sigma \gg 1$, their behavior is $\Delta_2 = 1 + \sigma/35 + \cdots$, $\tau_W^2/\tau_D = \sigma/70 + \cdots$, and $\Delta_2 = 1 + \sigma^{-1} + \cdots$, $\tau_W^2/\tau_D \sim -1/2\sigma + \cdots$, respectively. Thus, setting $\xi(t) = \xi \cos \omega t$, (C.15) yields

$$f_2^{(2)}(t) = \frac{\chi_2\xi^2}{2}\mathrm{Re}\left[\left(1 + \frac{\mathrm{e}^{2\mathrm{i}\omega\mathrm{t}}}{1 + 2\mathrm{i}\omega\tau_2^{\mathrm{eff}}}\right)\left(\frac{\Delta_2}{1 + \mathrm{i}\omega/\lambda_1} + \frac{1 - \Delta_2}{1 + \mathrm{i}\omega\tau_{\mathrm{W}}^2}\right)\right] \tag{C.17}$$

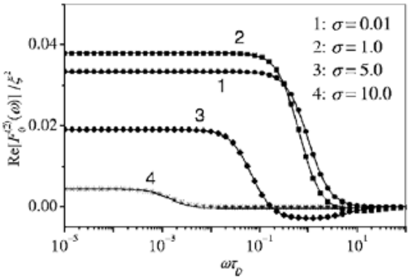

Fig. C.2. Exact Re $[\mathrm{F}_0^{(2)}(\omega)]/\xi^2$ (C.13, *solid lines*) and approximate ((C.17), *symbols*) solutions

Apparently, the KER calculated from the approximate equation (C.17) is in excellent agreement with the exact equation (C.13); see Figures C.2 and C.3. The results suggest a method of measuring the overbarrier relaxation time $1/\lambda_1$, i.e., the inverse Kramers escape rate, using the dc component of the Kerr response. For free

Table C.1. Numerical values of $(\lambda_1\tau_D)^{-1}$, τ^{eff}/τ_D, and τ/τ_D

σ	0	1	2	3	4	5	6	8	10
$(\lambda_1\tau_D)^{-1}$	1.0	1.531	2.476	4.243	7.702	14.77	29.75	135.8	693.9
τ^{eff}/τ_D	-1.0	-2.169	83.37	2.411	1.352	1.021	0.881	0.805	0.826
τ/τ_D	1.0	1.582	2.655	4.713	8.788	17.09	34.43	153.2	757.9

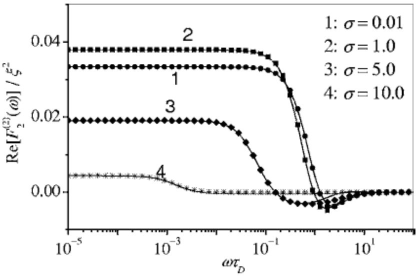

Fig. C.3. Exact Re $[\mathrm{F}_2^{(2)}(\omega)]/\xi^2$ (C.13, *solid lines*) and approximate ((C.17), symbols) *symbols*

diffusion ($\sigma = 0$), $\chi_2 = 1/15$, $\tau_2^{eff} = \tau_D/3$, $\lambda_1 = 1/\tau_D$, and $\Delta_2 = 1$ so that (C.17) reduces to the known results [122], [124].

Finally as in [122], [124], $f_1^{(1)}(t)$, and $f_2^{(2)}(t)$ yield the NLDE $f_1^{(3)}(t)$. We have

$$\begin{aligned} f_1^{(3)}(t) = -\frac{1}{6}\left(\langle P_1^4\rangle_0 - 3\langle P_1^2\rangle_0^2\right) &\int_{-\infty}^{t} \xi(t')\dot{\Phi}^{(3)}(t-t') \\ &\times \int_{-\infty}^{t'} \xi(t'')\dot{\Phi}_{2,2}(t'-t'') \\ &\times \int_{-\infty}^{t''} \dot{\Phi}^{(1)}(t''-t''')\xi(t''')\mathrm{d}t'''\mathrm{d}t''\mathrm{d}t' \end{aligned} \tag{C.18}$$

representing the generalization of (21) of [122] or (14.21) of [124] to a mean field. $\Phi^{(3)}(t)$ contains the contribution of the matrix elements of the KER to $f_1^{(3)}(t)$ and is represented by a two-mode approximation as the propagator involves overbarrier relaxation.

We have described exact and approximate calculations of the nonlinear orientational ac response of permanent dipoles in the presence of a uniaxial potential (C.1). The approximate calculation accurately represents the relevant matrix elements of the exact time-ordered matrix exponential solution generated by perturbation theory using Picard's method [122], [124], [331]. Thus the approximate solution effectively generalizes the existing analytic results for noninteracting dipoles in ac driving fields to a mean field potential and has a similar mathematical form (C.17) (but with parameters given in terms of the barrier height parameter σ), so explaining the successful application of the known frequency-dependence of the KER for free diffusion to the analysis of experimental spectra of electric birefringence of nematics which was previously done without any theoretical justification (see, e.g., [532]). The results apply to both nonlinear dielectric relaxation and KER of nematics, and magnetic birefringence relaxation of ferrofluids. The solution of the problem citing, for example, the matrix element $f_2^{(2)}(t)$, clearly demonstrates that the dc component of a second-order nonlinear response contains information about the linear response function. This fact suggests possible methods of measurement of the overbarrier relaxation time (inverse Kramers rate) via the dc electric or magnetic birefringence. We have illustrated the calculation for the simplest mean field potential and have ignored induced moments. The calculation may, however, be very easily extended to (a) nonstationary response, (b) induced moments, and (c) other mean field potentials such as biaxial anisotropy. Finally, the method may be extended to fractional Brownian motion resulting in anomalous relaxation as described in [142].

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