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Matrix Solution of a Diffusion Equation for Dielectric Relaxation

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Sack's diffusion equation calculations of relaxation effects in dielectrics based on a spherical model are simplified. The steady state response to an alternating field can be easily expressed as a series in powers of a dimensionless parameter by inverting a matrix.

Sack [1] investigated the rotational Brownian motion of a sphere with moment of inertia I and dipole moment μ , which is subject to a frictional couple $I\beta$ times the angular velocity and an electric field F in a fixed direction by writing down a diffusion equation for the probability density w in configuration-angular velocity space. He then put

$$\Psi = \exp\left(kT\sum_\ell u_\ell^2/2I\right)\iiint w(\theta,v_\theta,v_\phi,v_z,t)\exp\left(-i\sum_\ell u_\ell v_\ell\right)dv_\theta\, dv_\phi\, dv_z,$$

θ being the angle between the directions of the dipole axis and F, and deduced that

$$\frac{\partial\Psi}{\partial t}+i\frac{\partial^2\Psi}{\partial\theta\partial u_\theta}-\frac{iu_\theta}{I}\left[kT\frac{\partial\Psi}{\partial\theta}+\mu F\sin\theta\,\Psi\right]$$
$$+i\left[\cot\theta\frac{\partial}{\partial u_\phi}-\frac{\partial}{\partial u_z}-\frac{kT}{I}(\cot\theta\, u_\phi-u_z)\right]\left(u_\phi\frac{\partial\Psi}{\partial u_\theta}-u_\theta\frac{\partial\Psi}{\partial u_\phi}\right)=-\beta\sum_\ell u_\ell\frac{\partial\Psi}{\partial u_\ell}. \tag{1}$$

The subsequent calculations required for the study of relaxation effects in dielectrics may be considerably reduced by writing in the linear approximation for the steady state response to a field $F = F_0e^{i\omega t}$

$$8\pi^2\Psi = 1+e^{i\omega t}\Big\{\cos\theta\sum_{r=0}^{\infty}A_r\left(kT\sum_\ell u_\ell^2/2I\right)^r+\sin\theta\, u_\theta\sum_{r=0}^{\infty}B_r\left(kT\sum_\ell u_\ell^2/2I\right)^r$$
$$+(\cos\theta\, u_z^2+\sin\theta\, u_z u_\phi)\sum_{r=0}^{\infty}C_r\left(kT\sum_\ell u_\ell^2/2I\right)^r+\cdots\Big\} \tag{2}$$

and employing matrix methods for the solution of the equations for A_r, B_r, C_r that result from substituting (2) into (1). When A_r and C_r are eliminated, it is found that

$$(L+\gamma M)\begin{pmatrix}B_0\\B_1\\B_2\\\vdots\end{pmatrix}=\frac{i\mu F_0}{\beta I}\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}, \tag{3}$$

where

$$L = \begin{pmatrix} (1) & 0 & 0 & \cdots \\ 0 & (3) & 0 & \cdots \\ 0 & 0 & (5) & 0 \cdots \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad M = \begin{pmatrix} \frac{2}{(0)} + \frac{3}{(2)} & -\frac{1.5}{(2)} & 0 & \cdot & \cdot \\ -\frac{2}{(2)} & \frac{4}{(2)} + \frac{5}{(4)} & -\frac{2.7}{(4)} & 0 & \cdot \\ 0 & -\frac{2}{(4)} & \frac{6}{(4)} + \frac{7}{(6)} & -\frac{3.9}{(6)} & 0 \\ \cdot & 0 & \cdot & \cdot & \cdot \end{pmatrix}$$

and we have written

$$\frac{kT}{I\beta^2} = \gamma, \quad \frac{i\omega}{\beta} = (0), \quad 1 + \frac{i\omega}{\beta} = (1), \quad 2 + \frac{i\omega}{\beta} = (2), \text{ etc.}$$

If $P^*(\omega)e^{i\omega t}$ is the polarization of the sphere due to the field $F_0 e^{i\omega t}$ and P_0 is the polarization due to the constant field F_0, it may be shown that

$$\frac{P^*(\omega)}{P_0} = -\frac{2B_0 kT}{\mu F_0 \omega} = \frac{2\beta\gamma}{i\omega}\left((L+\gamma M)^{-1}\right)_{00},$$

by (3). On expanding the matrix as a series in powers of the dimensionless γ one gets

$$\frac{P^*(\omega)}{P_0} = \frac{2\beta\gamma}{i\omega}\left\{L^{-1}_{00} - \gamma(L^{-1}ML^{-1})_{00} + \gamma^2(L^{-1}ML^{-1}ML^{-1})_{00} - \gamma^3(L^{-1}ML^{-1}ML^{-1}ML^{-1})_{00} + \cdots\right\}. \quad (4)$$

Since L^{-1} is a diagonal matrix, the evaluation of the terms in the bracket is not difficult; it is in fact very much easier than finding the expansion in powers of γ for the continued fraction of Sack. The following is the explicit expression for (4) as far as the γ^5 - terms:

$$
\begin{aligned}
\frac{P^*(\omega)}{P_0} = {} & \frac{2\gamma}{(0)(1)} - \frac{2\gamma^2}{(0)(1)^2}\left\{\frac{2}{(0)} + \frac{3}{(2)}\right\} + \frac{2\gamma^3}{(0)(1)^2}\left\{\frac{4}{(0)^2(1)} + \frac{12}{(0)(1)(2)} + \frac{9}{(1)(2)^2} + \frac{10}{(2)^2(3)}\right\} \\
& - \frac{2\gamma^4}{(0)(1)^2}\left\{\frac{8}{(0)^3(1)^2} + \frac{36}{(0)^2(1)^2(2)} + \frac{54}{(0)(1)^2(2)^2} + \frac{40}{(0)(1)(2)^2(3)} \right. \\
& \qquad \left. + \frac{27}{(1)^2(2)^3} + \frac{60}{(1)(2)^3(3)} + \frac{40}{(2)^3(3)^2} + \frac{50}{(2)^2(3)^2(4)}\right\} \\
& + \frac{2\gamma^5}{(0)(1)^2}\left\{\frac{16}{(0)^4(1)^3} + \frac{96}{(0)^3(1)^3(2)} + \frac{216}{(0)^2(1)^3(2)^2} + \frac{120}{(0)^2(1)^2(2)^2(3)} \right. \\
& \qquad + \frac{216}{(0)(1)^3(2)^3} + \frac{360}{(0)(1)^2(2)^3(3)} + \frac{160}{(0)(1)(2)^3(3)^2} + \frac{200}{(0)(1)(2)^2(3)^2(4)} \\
& \qquad + \frac{81}{(1)^3(2)^4} + \frac{270}{(1)^2(2)^4(3)} + \frac{340}{(1)(2)^4(3)^2} + \frac{300}{(1)(2)^3(3)^2(4)} \\
& \qquad \left. + \frac{160}{(2)^4(3)^3} + \frac{400}{(2)^3(3)^3(4)} + \frac{250}{(2)^2(3)^3(4)^2} + \frac{280}{(2)^2(3)^2(4)^2(5)}\right\} \\
& - \ \cdots
\end{aligned}
$$

A recent calculation based on a Langevin equation [2] produced the above series as far as the terms of order γ^4 .

A more extensive account of the above investigations will be submitted elsewhere for publication.

References

[1] R. A. Sack "Relaxation Processes and Inertial Effects II. Free Rotation in Space", Proc. Phys. Soc. B70, 414-426, 1957.

[2] G. W. Ford, J. T. Lewis and J. McConnell "Graphical Study of Rotational Brownian Motion", Dublin Institute for Advanced Studies preprint No. DIAS-TP-75-52.