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COMMENT

Relaxation function for a system with a bounded broad distribution of relaxation times

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Abstract. The long-time limit of the relaxation function for system with a broad uniform but bounded continuous distribution of relaxation times is shown to be of the Yukawa form. This is in contrast to the single or multiple exponential functions often used to extract relaxation time constant τ from fitting experimental or numerical simulation data. Although such fittings will still obtained the correct τ in the long-time limit, our results predict a logarithmic term, which will slow the convergence.

Relaxation in complex, slowly relaxing, strongly interacting materials is not well understood and has been a topic of considerable physical interests for many years. Even in well defined simple dynamical lattice models near the critical point, understanding remained incomplete (see Hohenberg and Halperin 1977 for an extensive review). In the absence of exact analytical solutions to most physically interesting models, numerical simulation of relaxation phenomena plays an important role (see Binder and Kalos 1979 for reviews). Major contributions of numerical simulation are numerical data on the properties of the relaxation function (see Landau 1988 for a recent summary). These numerical results are analysed to extract behaviours of relaxation time constants for comparison with theoretical predictions. For the long-time properties in simple systems, one often assumes a single exponential relaxation characterized by one relaxation time constant τ. In practice, one often needs more than one exponential decay function to provide a good fit of the data over a reasonable range of simulation times. Furthermore, on physical grounds, a distribution of relaxation time $g(\tau)$ is expected to be relevant in many model systems (see, for a discussion, Kretschmer *et al* 1976).

In this short comment, we present a simple but non-trivial analytical calculation on the long-time relaxation function of systems with a broad uniform but bounded continuous distribution of relaxation times. To our knowledge, our results are new and predict an asymptotic relaxation of the Yukawa form parametrized by the upper bound of the broad distribution (τ_{max}). This is in contrast to the single exponential relaxation function and indicates that the relaxation time constants from such fits to data of systems with bounded uniform broad continuous distribution will converge to τ_{max} in the very long-time limit but with a logarithmic term, which will slow the convergence.

We consider a system with a normalized continuous uniform distribution of relaxation times, $g(\tau) = g_0 = 1/(\tau_{max} - \tau_{min})$ for τ between τ_{min} and τ_{max}. A picture of parallel relaxation is assumed and the relaxation function becomes

$$f(t) = \int_{\tau_{min}}^{\tau_{max}} g(\tau)\exp(-t/\tau)\,d\tau = \int_{\tau_{min}}^{\tau_{max}} 1/(\tau_{max} - \tau_{min})\exp(-t/\tau)\,d\tau. \qquad (1)$$

We consider a change of variable of $y = \tau_{max}/\tau$ and reversing the limit of the integration to obtain

$$f(t) = \tau_{max}/(\tau_{max} - \tau_{min}) \int_1^{(\tau_{max}/\tau_{min})} \exp(-(t/\tau_{max})y)/y^2 \, dy. \qquad (2)$$

Next, we take the limit of a very broad distribution with $\tau_{max}/\tau_{min} \to \infty$ with

$$f(t) = \int_1^{\infty} \exp(-(t/\tau_{max})y)/y^2 \, dy. \qquad (3)$$

This can be recognized as related to an exponential integral $E_n(x)$ with $n = 2$ and $(x = t/\tau_{max})$. $E_n(x)$ obeys the following inequality (see Abramowitz and Stegun 1970):

$$\exp(-x)/(x+n) < E_n(x) \leqslant \exp(-x)/(x+n-1). \qquad (4)$$

For $t > \tau_{max}$ or the large-x limit, we obtain the Yukawa form for the relaxation function,

$$f(t) = \exp(-t/\tau_{max})/(t/\tau_{max}). \qquad (5)$$

It is now clear that, if one were to extract τ_{max} from fitting data obeying equation 5 by assuming an exponential function, a logarithmic correction of $\ln(t/\tau_{max})/(t/\tau_{max})$ would slow the convergence toward the correct τ_{max} in the large-(t/τ_{max}) limit.

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