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1994 J. Phys.: Condens. Matter 6 1253

(http://iopscience.iop.org/0953-8984/6/6/027)

J. Phys.: Condens. Matter 6 (1994) 1253–1260. Printed in the UK

A theory of the time-dependent properties of Heisenberg spin chains at infinite temperature

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Received 18 October 1993

Abstract. A coupled-mode theory for the spin response function is used to calculate time-dependent properties of the classical spin chain at infinite temperature. The behaviour of the spin autocorrelation function is consistent with computer simulation data, in that the exponent of the time tail decreases on moving from intermediate to asymptotic time regions. Results for the spin response function and memory function in the two time regions are obtained by a combination of asymptotic analysis and numerical studies. For a large wavevector, near the zone boundary, the spin response function displays a very pronounced oscillatory time dependence. However, there is next to no structure in the corresponding spectral function, in accord with simulation data. The asymptotic analysis shows that, in the infinite-temperature limit, coupled-mode theory does not comply with usual hydrodynamic assumptions, a view that has also emerged from analysis of some of the computer simulation data.

1. Introduction

A recent flurry of work on the time-dependent properties of classical Heisenberg spin chains, a model of long-standing interest in statistical physics, is largely driven by reports of very extensive computer simulation studies (Müller 1989, Gerling and Landau 1989, 1990, de Alcantara Bonfim and Reiter 1992). Thus far, work on the interpretation of the computer simulation data (e.g. Böhm *et al* 1993, de Alcantara Bonfim and Reiter 1993) has not included a study of a theoretical model based on the coupled-mode approximation even though it has proved very successful in other contexts. Such a study is valuable for two main reasons. First, a confrontation of predictions based on the coupled-mode approximation and simulation data contributes to understanding the physical significance of the data. Second, it aids in an appreciation of the strengths and weaknesses of the coupled-mode approximation.

The version of the coupled-mode approximation at the heart of the present study has been shown to provide a good description of the low-temperature spin dynamics of a classical Heisenberg spin chain (Lovesey and Megann 1986). It is not sufficient to use the standard form of approximation (e.g. Lovesey 1986), because this does not contain the strong spin correlations that manifest themselves in collective excitations reminiscent of spin waves.

The refined coupled-mode theory of Lovesey and Megann (1986) appropriate for an infinite-temperature spin chain is discussed in section 4, following very brief accounts of the Heisenberg model and spin response function. Asymptotic properties of the spin response and memory functions are also provided in section 4. The intermediate time region, $1 \leqslant tJ \leqslant 10$, is investigated in section 5; appropriate approximate expressions for the memory and response functions are given. An analytic approximation to the memory function is explored in section 6. Our results are discussed in section 7, and placed in context with findings from computer simulation studies.

0953-8984/94/061253+08$07.50

2. Heisenberg model

The model consists of unit vectors S_j located at positions, labelled by the index j, that lie on a line to which periodic boundary conditions are applied. The Heisenberg Hamiltonian is

$$\mathcal{H} = -\frac{1}{2} J \sum_{j,\delta} S_j \cdot S_{j+\delta}. \tag{2.1}$$

At infinite temperatures, static and dynamic properties do not depend on the sign of the exchange coupling J between nearest-neighbour sites.

For classical spin variables the static spin correlation functions can be obtained in closed analytic form, even at a finite temperature. In the present study we need only record results for the second and fourth frequency moments of the frequency- and wavevector-dependent response function defined in (3.1). The required results for the normalized second (ω_0^2) and fourth (ω_l^2) frequency moments of a classical spin chain evaluated in the high-temperature limit are

$$\omega_0^2 = \tfrac{4}{3} J^2 (1 - \gamma_q) \tag{2.2}$$

$$\omega_l^2 = \tfrac{2}{3} J^2 (5 - 3\gamma_q). \tag{2.3}$$

Here, $\gamma_q = \cos q$, and the wavevector q is measured in units of the inverse of the interspin spacing, i.e. $-\pi \leqslant q \leqslant \pi$.

3. Response functions

Dynamic properties of the model (2.1) are studied in terms of spin correlation functions $\langle S_j^\alpha(0) S_{j'}^\beta(t)\rangle$ where α and β label Cartesian components, and $S(t)$ is the Heisenberg representation for the time (t) dependence of the spin variables. For a spatially isotropic spin–spin interaction, as in (2.1), the correlation function vanishes for $\alpha \neq \beta$, and for $\alpha = \beta$ it is independent of α; for simplicity of notation, we henceforth omit the Cartesian label in the correlation function. Since the spin variables are unit vectors,

$$\langle S_j(0) S_j(0)\rangle = \tfrac{1}{3}.$$

The response function of interest, denoted $G(q, t)$, is obtained from the spatial Fourier transform of S_j, which we write as S_q. Then

$$G(q, t) = \langle S_q(0) S_{-q}(t)\rangle \tag{3.1}$$

and the isothermal susceptibility, in the high-temperature limit is,

$$= (1/T) G(q, 0) = (1/3T). \tag{3.2}$$

The response function $G(q, t)$ is an even function of both q and t. The second and fourth time derivatives of $G(q, t)$ are proportional to ω_0^2 and ω_l^2; in our notation

$$G(q, t) = G(q, 0) \left\{1 - \frac{1}{2!} t^2 \omega_0^2 + \frac{1}{4!} t^4 \omega_0^2 \omega_l^2 - \ldots\right\}. \tag{3.3}$$

We will refer to this expression on many occasions.

4. Coupled-mode approximation for $G(q, t)$

The coupled-mode approximation for $G(q, t)$ is conveniently derived from the generalized Langevin equation for $S_q(t)$, which is a formally exact representation of the time development of the spin variable. In the language of the generalized Langevin equation, the standard coupled-mode approximation is derived from the exact formalism by making a straightforward approximation to the memory function, $K(q, t)$, the result of which is a closed set of equations for $G(q, t)$. The precise relation between $G(q, t)$ and $K(q, t)$ is

$$\partial_t G(q, t) = -\int_0^t \mathrm{d}t'\, K(q, t - t')G(q, t') \tag{4.1}$$

and the standard coupled-mode approximation for $K(q, t)$ is of the form

$$\sin^2(q/2) \int \mathrm{d}p \sin^2 p\, G(p + \tfrac{1}{2}q, t)G(p - \tfrac{1}{2}q, t). \tag{4.2}$$

Applied to one-dimensional magnets, this coupled-mode equation is inadequate because it does not reproduce the long-lived collective excitations, akin to spin waves, that exist at low temperatures. The failure contrasts with great success in the interpretation of critical and paramagnetic spin fluctuations in three-dimensional magnetic systems (Cuccoli *et al* 1989, 1990, Westhead *et al* 1991).

In view of the established shortcoming of (4.2) for one-dimensional magnets with $T \ll J$, we have minimal confidence in using it for the opposite limiting case $T \gg J$. Instead, we use the refined coupled-mode theory introduced by Lovesey and Megann (1986), which faithfully describes the dynamic properties of one-dimensional magnets at $T \ll J$. The refinement takes the form of renormalizing the interactions accounted for in the coupled-mode approximation, in such a way that they adequately describe the strongly correlated spin state that exists for $T \ll J$. In a wider context, the renormalization procedure was earlier developed by Martin and coworkers (1973).

Taking the limit $(T/J) \to \infty$ in the equation derived by Lovesey and Megann (1986),

$$K(q, t) = (24/\pi)\sin^2(q/2) \int_{-\pi}^{\pi} \mathrm{d}p \sin^2 p\, G(p + \tfrac{1}{2}q, t\mu_q)G(p - \tfrac{1}{2}q, t\mu_q) \tag{4.3}$$

where we have set $J = 1$, and

$$\mu_q = \tfrac{1}{2}(3 - \gamma_q)^{1/2}. \tag{4.4}$$

One feature of (4.3) is that it is consistent with (3.3), e.g. $K(q, 0) = \omega_0^2$. Equations (4.1), (4.3) and (4.4) constitute the refined coupled-mode approximation for one-dimensional magnets at infinite temperature. In the high-temperature limit, the only difference between the standard and refined theories is the factor μ_q in the latter; for the standard theory $\mu_q = 1$ for all wavevectors (and temperatures). One effect of μ_q is to make the refined theory consistent with the fourth frequency moment (2.3).

Asymptotic properties ($q \to 0$, $t \to \infty$, $q^2 t \to 0$) of the response and memory function are obtained from consideration of homogeneous forms

$$\begin{aligned} K(q, t) &= \lambda K(q\lambda^a, t\lambda^b) \\ G(q, t) &= G(q\lambda^a, t\lambda^b) \end{aligned} \tag{4.5}$$

taken in the limit $\lambda^a \to 0$. These forms for K and G have not been shown to be valid for arbitrary values of the arguments. One finds by analysis, $a = -\frac{1}{5}$, $b = \frac{1}{2}$, and

$$K(q, t) = q^5 f(tq^{5/2}) \qquad G(q, t) = g(tq^{5/2}) \tag{4.6}$$

where the functions $f(x)$ and $g(x)$ are determined by coupled integral equations derived from (4.2) and (4.3). The precise form of these functions is not required to obtain the asymptotic time dependences of $K(q,t)$, namely

$$K(q,t) \sim (1/t)^{6/5}. \tag{4.7}$$

The spin autocorrelation function $\langle S_j(0)S_j(t)\rangle$ is proportional to the integral of $G(q,t)$ with respect to q, and the asymptotic time dependence is found to be

$$\langle S_j(0)S_j(t)\rangle \sim (1/t)^{2/5}. \tag{4.8}$$

The intermediate time development of $K(q,t)$ and $G(q,t)$—intermediate between the expansion (3.3) and the foregoing asymptotic behaviour—is explored in the next section.

5. Intermediate time dependence of $K(q,t)$ and $G(q,t)$

The numerical solution of (4.1) and (4.3) is displayed in figures 1 and 2 for $0 < t < 10$ (t is always in units of $1/J$). Tests of our iteration scheme included a stringent comparison between the analytic expression for G and numerical values derived for the special case $K \propto \exp(-t/\tau)$. Our reported results were obtained using meshes in q and t space with elements of size $(\pi/20)$ and $(0.01/J)$, respectively.

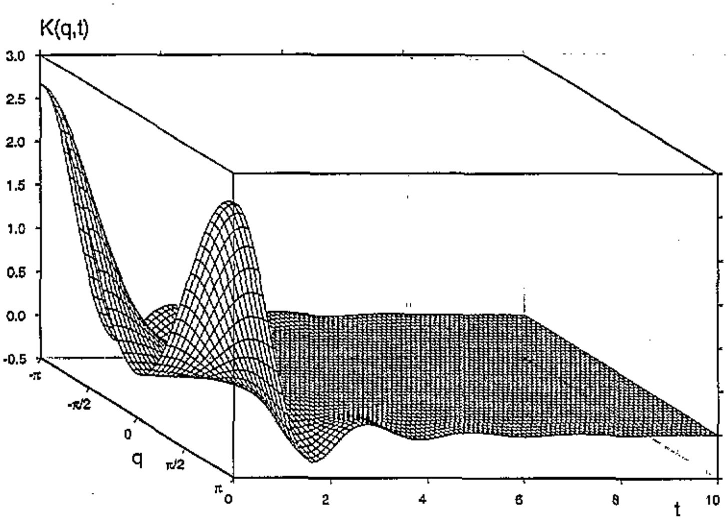

Figure 1. The memory function, $K(q,t)$, obtained from (4.1), (4.3) and (4.4) is displayed for $-\pi \leqslant q \leqslant \pi$ and $0 \leqslant t \leqslant 10$. The units are $J = 1$, and unit spacing between neighbouring spins in the chain.

The memory and response functions are radically different, e.g. $K(0,t) = 0$, and $G(q,0) = \frac{1}{3} = G(0,t)$. Oscillations in the memory function die out more rapidly than those in the response function, as expected. For q at the zone boundary both functions show pronounced oscillations with a common frequency. However, the damping in $G(\pi,t)$ is sufficiently strong to smooth out structure in the corresponding frequency spectrum, shown in figure 3, which is, in fact, proportional to the inelastic neutron scattering cross-section. Even so, the frequency spectrum is significantly different from a Gaussian approximation obtained by the Fourier transform of $\exp(-\frac{1}{2}t^2\omega_0^2)$ that is consistent with the first two terms in (3.3).

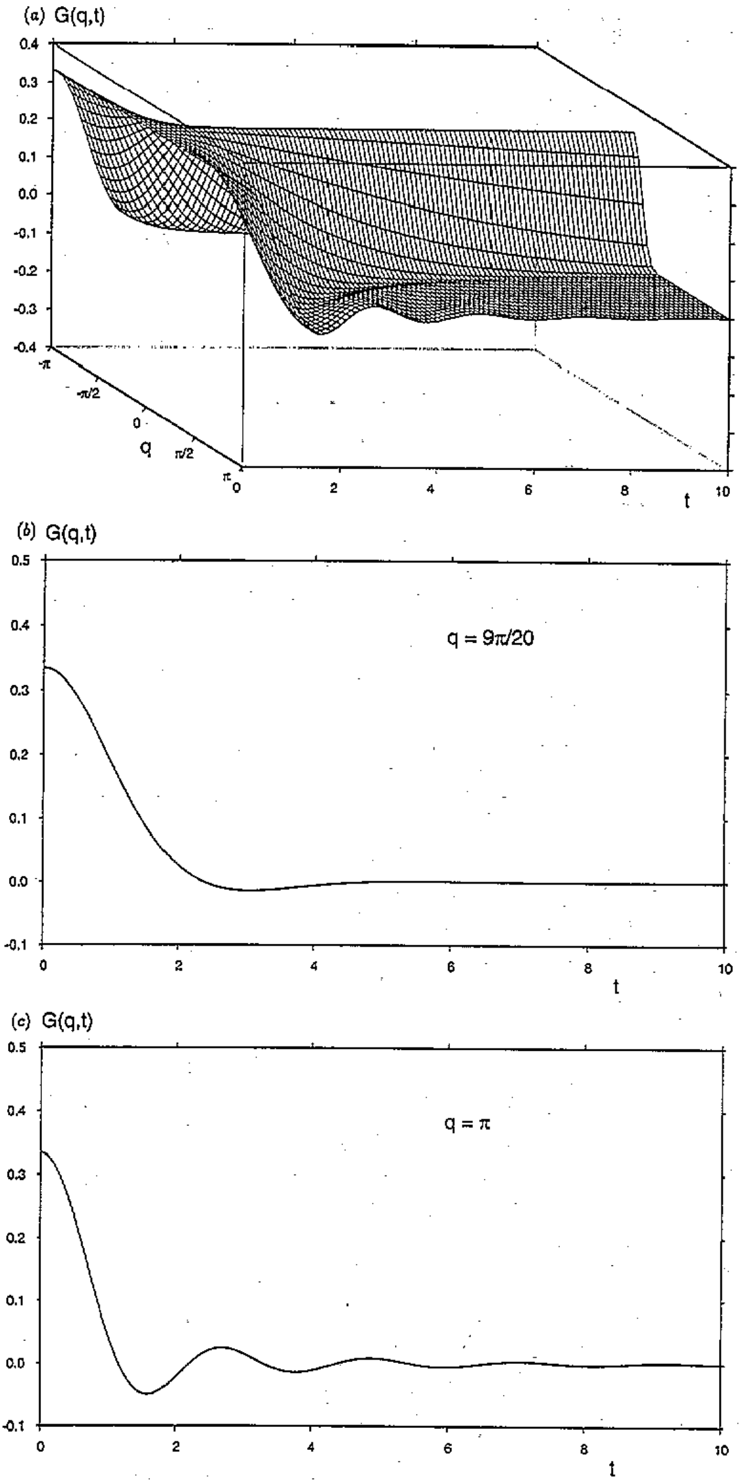

Figure 2. The response function, $G(q, t)$, that corresponds to the memory function displayed in figure 1. (*a*) provides a survey of the function, and (*b*) and (*c*) give more detail of the time evolution.

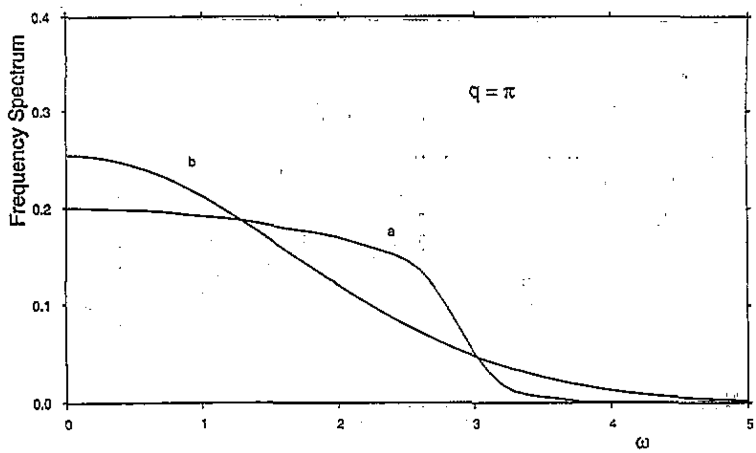

Figure 3. The time Fourier transform of $G(q,t)$ displayed in figure 2(c) is shown together with the Gaussian model $\alpha\exp(-\omega^2/2\omega_0^2)$; they are labelled a and b, respectively.

Analysis of the numerical results for $K(q,t)$ and $G(q,t)$ for small values of ($q \leqslant \pi/10$) shows that, with $t > 1$, the memory function is proportional to $(1/t)^2$ while the response function decays exponentially with time. These observations, together with (4.1), lead to the following approximate forms for the functions, valid at intermediate times:

$$\begin{aligned} G(q,t) &\sim \tfrac{1}{3}\exp(-tq^{3/2}\Gamma_0) \\ K(q,t) &\sim \left(\frac{4}{9\pi}\right)(q/t\Gamma_0)^2 \end{aligned} \tag{5.1}$$

where $\Gamma_0 \simeq 0.56$. The expression for $G(q,t)$ implies that the spin autocorrelation function at intermediate times decreases with a power law $(1/t)^{2/3}$.

6. Approximate memory function

There is some merit in exploring the use of an approximation to the memory function, if only to gauge the sensitivity of $G(q,t)$ to features in $K(q,t)$. To this end we have calculated an approximation to the memory function, denoted by $K_0(q,t)$, from (4.3) using for the response function

$$G(q,t) \sim G_0(q,t) = \tfrac{1}{3}\exp(-\tfrac{1}{2}t^2\omega_0^2)\{1 + \tfrac{1}{4}\omega_0^2(\omega_l^2 - 3\omega_0^2)t^4\}. \tag{6.1}$$

This expression is consistent with (3.3). The coefficient $(\omega_l^2 - 3\omega_0^2)$ changes sign at $\gamma_q = \frac{1}{3}$, and this is a signature for the oscillatory time behaviour of $G(q,t)$ which sets in with increasing values of q, cf figures 2(b) and (c).

Substituting $G_0(q,t)$ in (4.3) leads to

$$\begin{aligned} K_0(q,t) = &\left(\frac{16}{3z}\right)\sin^2(q/2)I_1(z)\exp(-\alpha) \\ &\times\{1 + \tfrac{1}{4}\alpha^2[-\tfrac{5}{2} + \tfrac{3}{2}\gamma_q + 4L_1\cos(q/2) - 3\gamma_q L_2]\}. \end{aligned} \tag{6.2}$$

In this expression, $\alpha = \frac{4}{3}(t\mu_q)^2$, $z = \alpha\cos(q/2)$, $I_n(z)$ is a modified Bessel function of the first kind, and the functions L_1 and L_2 are given by

$$L_1 = (z/I_1)(I_1/z)' \qquad L_2 = (z/I_1)(I_1/z)''$$

in which $I_1' = I_0$. Looking at figures 4 and 1 for $K_0(q,t)$ and the full memory function there are some significant differences, e.g. there is just one oscillation in K_0. It is, perhaps, a surprise that the corresponding response functions are similar in all respects, as can be seen by looking at figures 5 and 2(a).

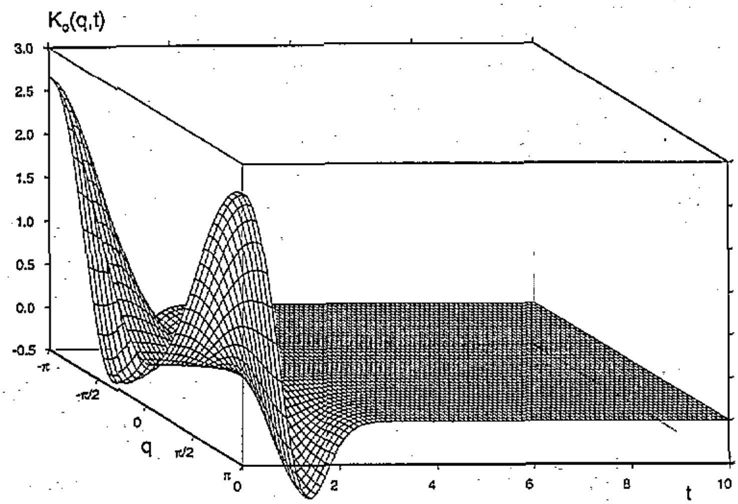

Figure 4. $K_0(q, t)$ defined in (6.2).

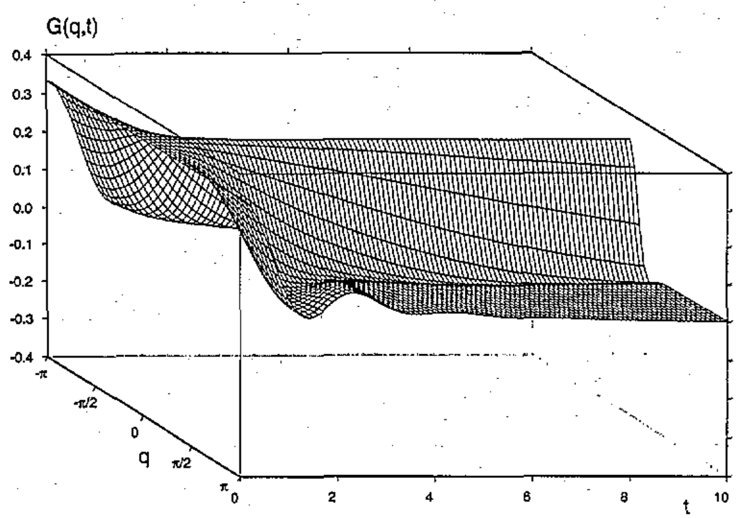

Figure 5. The response function obtained from (4.1) using the memory function $K_0(q, t)$.

7. Discussion

The work reported provides a rather complete survey of the time-dependent properties of the classical spin chain at infinite temperature by utilizing a refined version of the standard coupled-mode approximation.

It is possible to make contact on several issues with results obtained from the computer simulation studies mentioned in section 1. First, the frequency spectrum shown in figure 3 is completely consistent with data on the same function reported by Gerling and Landau (1990). We find no evidence in the frequency spectrum of a distinct contribution from the oscillatory time dependence evident in $G(q, t)$ when q is near the zone boundary. The discussion in section 6 gives some understanding of the onset of the oscillatory behaviour in $G(q, t)$ with increasing q.

Turning next to the spin autocorrelation function $\langle S_j(0) S_j(t)\rangle$, we find $(1/t)^{2/3}$ and $(1/t)^{2/5}$ in the intermediate and asymptotic time regions. Work by Müller (1989) and

Gerling and Landau (1989, 1990) provides convincing evidence of a very pronounced non-asymptotic time regime in which the exponent for the time tail decreases. For short times, Gerling and Landau (1990) report an exponent well above 0.6, but this decreases systematically as the data analysis is moved to longer time intervals, and extrapolates to a value close to 0.5, which appears to be significantly larger than the value of $\frac{2}{5}$ obtained from coupled-mode theory. On the question of the existence of spin diffusion, note that the spin diffusion constant is proportional to

$$\frac{1}{q^2}\int_0^\infty \mathrm{d}t \exp(-st)K(q,t)$$

evaluated with the limits $q \to 0$, followed by $s \to 0$. The intermediate and asymptotic time behaviour we find for $K(q,t)$, at small q, implies that the diffusion constant is indeed finite.

Finally, the asymptotic behaviour of $G(q,t)$ shown in (4.6) demonstrates that, in the infinite-temperature limit, coupled-mode theory is not consistent with the usual hydrodynamic assumptions. Such a view has also emerged from an analysis by de Alcantara Bonfim and Reiter (1992, 1993) of computer simulation data but, at present, there is no consensus of opinion on the topic (Böhm *et al* 1993).

Note added in proof. Böhm and Leschke have extended their analysis based on the calculation of many frequency moments and thereby improved the interpretation of computer simulation data: (1993) *Physica* A **199** 116.

Acknowledgment

One of us (EB) is grateful to the Director of the Rutherford Appleton Laboratory for facilities used in the course of the work.

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