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# A THREE-PARAMETER GRAM-CHARLIER GAUSSIAN REPRESENTATION OF THE SPECTRAL FUNCTION OF SPIN CORRELATIONS

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A possible three-parameter Gram-Charlier form of the Gaussian diffusivity representation of the magnetic spin spectral function is evaluated for a restricted XY Heisenberg model, a linear chain of $S = \frac{1}{2}$ spins with only transverse exchange at elevated temperature. A brief analytical background is presented for the method of wave-vector-dependent frequency moments, which are used to determine the approximate spectral function. The three-parameter form of the spectral function is compared with a previous corresponding two-parameter form and with an exact solution available for the restricted XY model. It is concluded that the postulated three-parameter Gram-Charlier Gaussian diffusivity, utilizing the additional information in the sixth frequency moment, offers a definite improvement in the representation of spin spectral functions and correlations.



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# A THREE-PARAMETER GRAM-CHARLIER GAUSSIAN REPRESENTATION OF THE SPECTRAL FUNCTION OF SPIN CORRELATIONS

by

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## INTRODUCTION

A phenomenological approach to the time dependence of spin correlations has been successfully based on a two-parameter Gaussian approximation for the generalized diffusivity.[1-5] This method, valid for slowly varying disturbances, i.e., small frequencies and wave-vectors, relates the behavior of spin correlations to a hydrodynamic description of the diffusion of the magnetization density in equilibrium.[1,6] This method circumvents the calculational difficulties involved in the direct approach of perturbation and diagrammatic techniques for describing the collision-like process by requiring, instead, the computation of wave-vector-dependent frequency moments of the spectral function of the spin correlation to any desired order in a high-temperature expansion.

The principal objective of this paper is to extend the use of the Gaussian diffusivity approximation of the spectral function to a three-parameter form of the Gram-Charlier type. Since the knowledge of the first three non-vanishing frequency moments $\langle \omega^n \rangle_{\vec{K}}$, n = 0, 2, and 4, establishes a two-parameter representation of the spectral function, a three-parameter form requires the further determination of the sixth moment $\langle \omega^6 \rangle_{\vec{K}}$. Therefore, in Heisenberg spin systems for which sixth moment calculations are available or can be easily obtained, it is reasonable to expect an improved representation of spin correlations with a three-parameter form of the diffusivity, utilizing the additional information contained in the sixth moment. Although a pertinent sixth-moment calculation for the isotropic Heisenberg paramagnet at elevated temperatures with arbitrary spin and arbitrary range of the exchange interactions was attempted in a laborious computation,[7] subsequent investigations uncovered certain errors in the result. Therefore, this assessment of the three-parameter Gram-Charlier Gaussian is directed toward a simpler spin system the restricted XY model for which Katsura et al.[8] have obtained the dynamic properties by using the fermion Green function method.

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## FORMULATION

In the XY model no exchange coupling exists between the z components of the spins while the x and y components are bilinearly coupled among themselves by pairwise exchange potentials. The restricted XY model is considered to be a system with only nearest-neighbor XY exchange at infinite temperature and with $S = \frac{1}{2}$ spins distributed along a linear chain. For this model the exact solution of the longitudinal spectral function $F^{zz}(\vec{K}, \omega)$, determined in the limit of high temperature,[8] can be used as a basis of comparison with various phenomenological forms of the spectral function utilizing the appropriate number of infinite-temperature frequency moments. The exact longitudinal spectral function, given as the imaginary part of the high-temperature wave-vector dependent susceptibility, is

$$F^{zz}(\vec{K}, \omega) = \frac{\beta\omega}{4\pi} \left\{ \left[ 4 I_+ \sin\left(\frac{K}{2}\right) \right]^2 - \omega^2 \right\}^{-\frac{1}{2}}$$

$$\text{for } |\omega| < 4 I_+ \sin\left(\frac{K}{2}\right)$$

$$= 0 \qquad ;\text{otherwise} \tag{1}$$

Here $\vec{K}$ is the reduced wave-vector, $\omega$ is the frequency, $I_+$ is the nearest neighbor XY (transverse) exchange, and $\beta = (kT)^{-1}$, where k is the Boltzmann constant the T is the absolute temperature. The Dirac system of units with $\hbar = 1$ is used.

The relevant Hamiltonian for the restricted XY model is

$$H = -\sum_{gp} I_+(gp)\left(S_g^x S_p^x + S_g^y S_p^y\right) \tag{2}$$

where, e.g., $S_g^x$ is the x component of the spin vector associated with the lattice point g, and $I_+(gp)$ is the XY exchange interaction integral between sites g and p, such that $I_+(gg) = I_+(pp) = 0$.

The space-time dependent, longitudinal spin correlation function under the assumption of cylindrical symmetry is

$$F^{zz}(g - p, t - t') = \left\langle \left[ S_g^z(t), S_p^z(t') \right] \right\rangle \tag{3}$$

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8. S. Katsura, T. Horiguchi, M. Suzuki, Physica 46, 67 (1970).

with the spin operators in the Heisenberg picture. Here the angular brackets denote a statistical thermal average over a canonical ensemble and the straight brackets denote a commutator. The Fourier representation of the spin correlation function is the spectral function

$$F^{zz}(\vec{K}, \omega) = \sum_{\vec{g}-\vec{p}} \frac{e^{-i\vec{K}\cdot(\vec{g}-\vec{p})}}{2\pi} \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega(t-t')}\, F^{zz}(g-p, t-t') \tag{4}$$

where the summation consists of N allowed wave-vectors falling within the first Brillouin zone. The symmetry properties of the spectral function show that it is even in $\vec{K}$ and odd in $\omega$. It has been shown[3] that the Fourier transform of the statistical correlation function is given by

$$\left\langle S^z_g(t)\, S^z_p(t') \right\rangle_\omega = \frac{1}{N} \sum_{\vec{K}} e^{i\vec{K}\cdot(\vec{g}-\vec{p})} \frac{F^{zz}(\vec{K}, \omega)}{1 - e^{-\beta\omega}} \tag{5}$$

The definition of the longitudinal frequency moments of the spectral function for integer n is

$$\langle \omega^n \rangle^{zz}_{\vec{K}} = \int_{-\infty}^{\infty} F^{zz}(\vec{K}, \omega)\, \omega^{n-1}\, d\omega \tag{6}$$

The odd moments vanish since the spectral function is odd in the frequency. An alternate form of the frequency moments is

$$\langle \omega^n \rangle^{zz}_{\vec{K}} = \sum_{\vec{g}-\vec{p}} e^{-i\vec{K}\cdot(\vec{g}-\vec{p})} \left[ \left( i\frac{d}{dt} \right)^r \left( -i\frac{d}{dt'} \right)^{n-1-r} F^{zz}(g-p, t-t') \right]_{t=t'} \tag{7}$$

where the indices n and r are non-negative integers such that n-1 > r and the sum over all position vectors $\vec{g}-\vec{p}$ includes the origin. This latter form of the frequency moments in Equation (7) is generally used in direct calculations of systems with more complex Hamiltonians by repeatedly applying the equation of motion

$$i\frac{d}{dt} S^z_g(t) = \left[ S^z_g(t), H \right] \tag{8}$$

3. R.A. Tahir-Kheli, Phys. Rev. 159, 439(1967); J. Appl. Phys. 40, 1550(1969).

and by using the high-temperature expansion procedure for the statistical thermal average

$$\langle(\ \ )\rangle = \mathrm{Tr}\left[e^{-\beta H}(\ \ )\right] \Big/ \mathrm{Tr}\left[e^{-\beta H}\right] \tag{9}$$

The generalized diffusivity $D^{zz}(\vec{K}, \omega)$ is introduced to represent the spin and spectral correlation functions for mathematical convenience. This phenomenological representation is generally less hazardous in its application than the often singular spectral function and reduces to a hydrodynamic limit for small wave-vectors and frequencies.[6]

The retarded double-time Green function

$$M^{zz}_{gp}(t-t') = -i\theta(t-t')\left\langle\left[S^z_g(t), S^z_p(t')\right]\right\rangle \tag{10}$$

where $\theta$ is the unit step function, has the well-known spectral representation[9]

$$M^{zz}(\vec{K}, \phi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{F^{zz}(\vec{K}, \omega)}{\phi - \omega} d\omega \tag{11}$$

where $M^{zz}(\vec{K}, \phi)$ is the analytic extension of the Fourier transform $M^{zz}(\vec{K}, \omega)$ of Equation (10), similar to the form of Equation (4), into the upper half of the complex frequency plane.

The generalized diffusivity $D^{zz}(\vec{K}, \omega)$ can now be defined in the relation

$$M^{zz}(\vec{K}, \phi) = M^{zz}(\vec{K}, 0)\left[1 - \left(1 - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{D^{zz}(\vec{K}, \omega)}{\phi^2 - \omega^2} d\omega\right)^{-1}\right] \tag{12}$$

If the diffusivity moments are defined as

$$\left\langle D^{2u}\right\rangle^{zz}_{\vec{K}} = \frac{1}{\pi}\int_{-\infty}^{\infty} D^{zz}(\vec{K}, \omega)\, \omega^{2u}\, d\omega \tag{13}$$

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6. L.P. Kadanoff and P.C. Martin, Ann. Phys. (N.Y.) 24, 419(1963).
9. D.N. Zubarev, Soviet Phys. — Usp. 3, 320(1960).

where u is an integer, then performing large $\phi$ expansions on Equations (11) and (12) yields the relations between the first few diffusivity moments and frequency moments, i.e.

$$\left\langle \omega^2 \right\rangle_{\vec{K}}^{zz} \Big/ \left\langle \omega^0 \right\rangle_{\vec{K}}^{zz} = \left\langle D^0 \right\rangle_{\vec{K}}^{zz} \tag{14a}$$

$$\left\langle \omega^4 \right\rangle_{\vec{K}}^{zz} \Big/ \left\langle \omega^0 \right\rangle_{\vec{K}}^{zz} = \left\langle D^2 \right\rangle_{\vec{K}}^{zz} + \left( \left\langle D^0 \right\rangle_{\vec{K}}^{zz} \right)^2 \tag{14b}$$

$$\left\langle \omega^6 \right\rangle_{\vec{K}}^{zz} \Big/ \left\langle \omega^0 \right\rangle_{\vec{K}}^{zz} = \left\langle D^4 \right\rangle_{\vec{K}}^{zz} + 2 \left\langle D^0 \right\rangle_{\vec{K}}^{zz} \left\langle D^2 \right\rangle_{\vec{K}}^{zz} + \left( \left\langle D^0 \right\rangle_{\vec{K}}^{zz} \right)^3 \tag{14c}$$

where it has been noted that

$$M^{zz}(\vec{K}, 0) = -\frac{1}{2\pi} \left\langle \omega^0 \right\rangle_{\vec{K}}^{zz} \tag{15}$$

Equations (11) and (12) also specify the following explicit relationship between the spectral function $F^{zz}(\vec{K}, \omega)$ and the diffusivity $D^{zz}(\vec{K}, \omega)$

$$\frac{F^{zz}(\vec{K}, \omega)}{\omega} = \frac{-2M^{zz}(\vec{K}, 0)\, D^{zz}(\vec{K}, \omega)}{\omega^2 \left( 1 + P \int_{-\infty}^{\infty} \frac{d\phi}{\pi} \frac{D^{zz}(\vec{K}, \phi)}{\phi^2 - \omega^2} \right)^2 + \left[ D^{zz}(\vec{K}, \omega) \right]^2} \tag{16}$$

where P denotes the principal part. Equation (16) is the final form of the approximate spectral function based on the diffusivity method.

The remaining necessary information is the specification of the functional form of the diffusivity. A three-parameter Gaussian in the Gram-Charlier form

$$D^{zz}(\vec{K}, \omega) = \Delta(\vec{K})\, \Gamma(\vec{K}) \exp\left\{ -\left[ \Gamma(\vec{K})\, \omega \right]^2 \right\} \left\{ 1 + b(\vec{K}) \left[ 4\Gamma^4(\vec{K})\, \omega^4 - 12\Gamma^2(\vec{K})\, \omega^2 + 3 \right] \right\} \tag{17}$$

is selected, with its relevant feature of computational convenience as an appropriate representation of the generalized diffusivity. Solving for the three lowest-order non-vanishing diffusivity moments of Equation (13), one obtains

$$\langle D^0 \rangle^{zz}_{\vec{K}} = \Pi^{-1/2}\,\Delta(\vec{K}) \tag{18a}$$

$$\langle D^2 \rangle^{zz}_{\vec{K}} = \Delta(\vec{K}) \Big/ \left[2\Pi^{1/2}\,\Gamma^2(\vec{K})\right] \tag{18b}$$

$$\langle D^4 \rangle^{zz}_{\vec{K}} = 3\Delta(\vec{K})\left[1 + 8b(\vec{K})\right] \Big/ \left[4\Pi^{1/2}\,\Gamma^4(\vec{K})\right] \tag{18c}$$

The three parameters $\Delta(\vec{K})$, $\Gamma(\vec{K})$, and $b(\vec{K})$ are directly calculated from the frequency moments through Equations (14), thereby avoiding reiterative processes.

The longitudinal frequency moments of the restricted XY model as determined by Equations (1) and (6), become

$$\langle \omega^0 \rangle^{zz}_{\vec{K}} = \tfrac{1}{4}\beta \tag{19a}$$

$$\langle \omega^2 \rangle^{zz}_{\vec{K}} = 2\beta\left[I_+ \sin(\tfrac{1}{2}K)\right]^2 \tag{19b}$$

$$\langle \omega^4 \rangle^{zz}_{\vec{K}} = 24\beta\left[I_+ \sin(\tfrac{1}{2}K)\right]^4 \tag{19c}$$

$$\langle \omega^6 \rangle^{zz}_{\vec{K}} = 320\beta\left[I_+ \sin(\tfrac{1}{2}K)\right]^6 \tag{19d}$$

These frequency moments agree with the appropriate limiting forms of the moments previously derived for an anisotropic Heisenberg paramagnet with arbitrary spin, arbitrary range of the exchange interactions, and arbitrary dimensionality.[4]

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4. R.A. Tahir-Kheli and D.G. McFadden, Phys. Rev. 178, 800(1969); 182, 604(1969); B-1, 3178(1970); B-1, 3649(1970).

## APPLICATION TO RESTRICTED XY MODEL

The approximate longitudinal spectral function based on the three-parameter Gram-Charlier Gaussian is therefore computed for the restricted XY model by Equation (16) with Equations (14), (15), and (17) — (19). In Figure 1 this result is given as a function of frequency in reduced units[4] and (for several values of the wave-vector) is compared with the exact spectral function of Equation (1) and with the corresponding two-parameter form, i.e., Equation (17) with b $(\vec{K}) = 0$. The exact results are indicated by the solid curves with the sharp divergences; the three-parameter Gram-Charlier results, by the non-diverging solid curves with rounded-off maxima; and the two-parameter results, by the dashed curves. It is seen that the three-parameter results are significantly better approximations to the exact results than the corresponding two-parameter results.

The frequency Fourier transforms of the longitudinal self-correlation function are calculated by Equation (5) at infinite temperature for the three formulations of the spectral function. These results in reduced units are displayed as functions of frequency in Figure 2. Here the quantity, a, denotes the factor $(\frac{1}{3})S(S+1)$, where $S = \frac{1}{2}$. The three-parameter Gram-Charlier Gaussian is seen to yield a slightly better representation of the exact results, as compared with the two-parameter Gaussian, although the expectation that the improvement in the fit might be greater is not completely fulfilled because of the region where the hump of the two-parameter curve crosses over the exact curve.

## FINAL REMARKS

Therefore, it is concluded that the three-parameter Gram-Charlier Gaussian diffusivity, utilizing the additional interaction information contained in the sixth frequency moment, does offer a substantial improvement in the representation of spin spectral functions and correlations as evidenced by the application to the restricted XY model. It is hoped that this present formulation can be equally applicable to more generalized spin systems for which reliable exact solutions are not presently available, but for which calculations of the various frequency moments may be more feasible.

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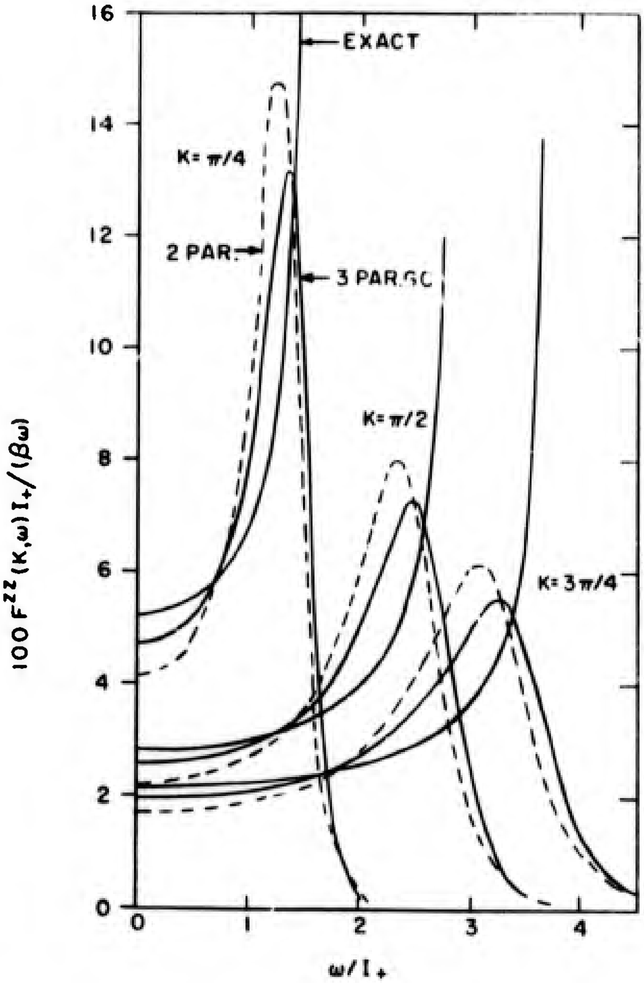
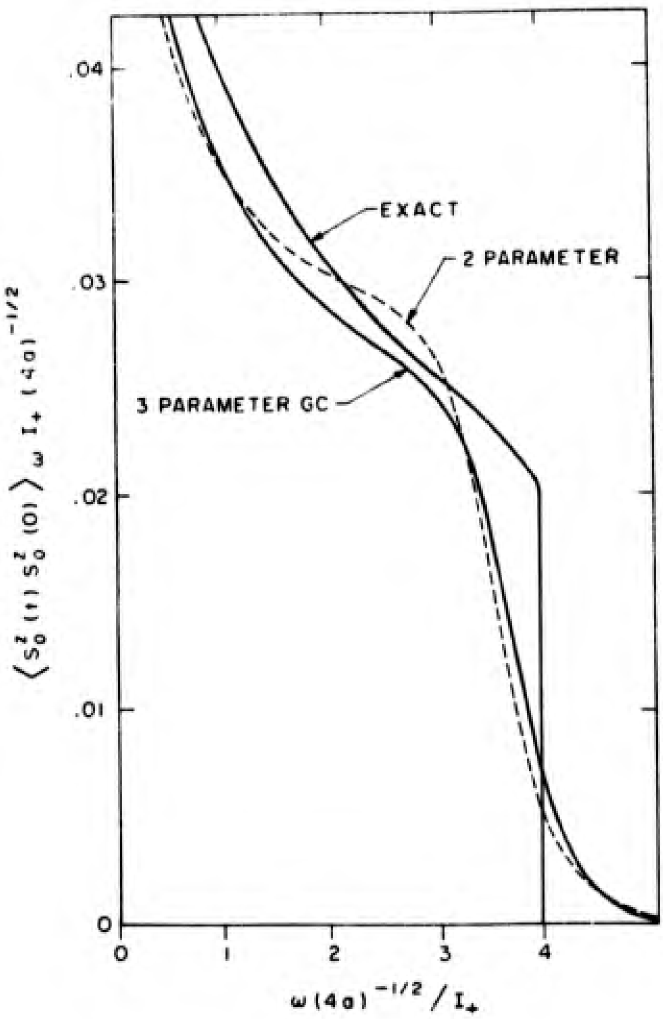



NOTE: The solid curves with the sharp divergences are the exact results of Equation 1. The solid curves with the maxima are the approximate spectral functions based on the three-parameter Gram-Charlier (GC) Gaussian diffusivity, as given in Equations 16 and 17. The dashed curves are similar results calculated for a corresponding two-parameter Gaussian diffusivity; i.e., Equation 17 with a third parameter $b(\vec{K})$ vanishing. Results are displayed for the wave-vector $\vec{K} = m\,\pi/4$ with m = 1, 2, and 3.

Figure 1. The Longitudinal Spectral Functions of the Restricted XY Model vs. Reduced Frequency




NOTE: The three forms of the spectral function as used in Figure 1 are also applied here. The solid curve with the cutoff represents the exact result; the other solid curve, the three-parameter GC Gaussian result; and the dashed curve, the two-parameter Gaussian result. The factor $a = (\frac{1}{3})S(S + 1)$, with $S = \frac{1}{2}$.

Figure 2. The Frequency Fourier Transforms of the Longitudinal Self-correlation Functions of the Restricted XY Model vs. Reduced Frequency

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