Remarks on the Fernandez-Gersch Procedure for Constructing Paramagnetic Line Shapes

F. A. MALINOSKI*

U. S. Army, Frankford Arsenal, Philadelphia, Pennsylvania 19137

AND

RAZA A. TAHIR-KHELI†

Department of Physics, Temple University, Philadelphia, Pennsylvania 19122

(Received 9 June 1970)

The Fernandez-Gersch procedure for constructing paramagnetic line shapes by the use of suitably weighted Lorentzian (L) and Gaussian (G) forms is analyzed. It is concluded that in practice the possible arbitrariness of their original suggestion regarding the weighting factors of the L and G forms is likely to be quite innocuous. Similarly, the straightforward embellishment of their Gram-Charlier series, to a form which does not violate the non-negativity requirement, does not lead to any noticeably superior results.

The suggestion[1] of Fernandez and Gersch (FG) to construct the frequency–wave-vector Fourier transform of the paramagnetic spin-correlation function from a suitably weighted combination of Lorentzian and Gaussian line shapes was recently shown[2] to lead to a fairly satisfactory representation of the line shape for a one-dimensional Heisenberg spin system.

The features of the line shape were obtained by

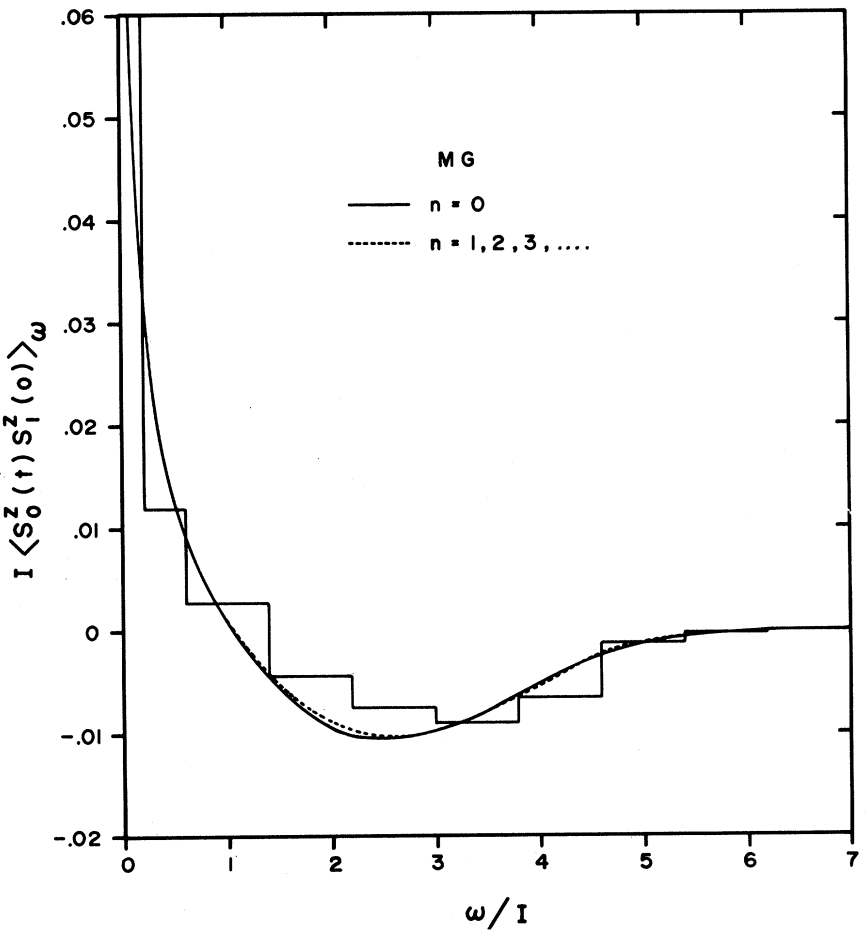

FIG. 1. Fourier transform of the first-nearest-neighbor spin ($S=\frac{1}{2}$) correlations at infinite temperature with different n indices in the weighting factors $W_n^{\pm}(K)$. For optimizing the usefulness of these figures we have used the MG procedure only. For higher spin magnitudes, the results for different values are even closer to each other than for $S=\frac{1}{2}$ shown here. (See Ref. 2 and the text for further explanation.)

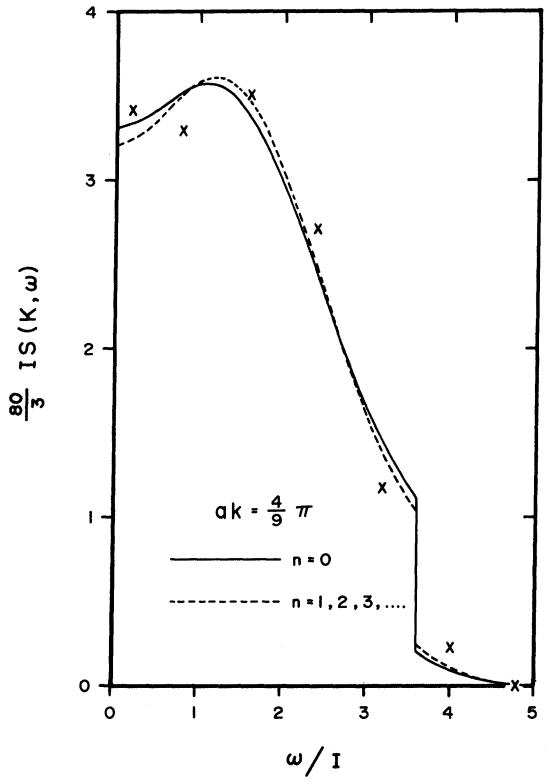

FIG. 2. Spin ($S=\frac{1}{2}$) spectral function $S(K,\omega)$ for $aK=4\pi/9$ for different n values. (See Ref. 2 for further explanation).

splitting the spectral function,

$$S(K,\omega)=\frac{3}{2\pi}\sum_R\int_{-\infty}^{\infty}\exp(-i\omega t-iK\cdot R)\times\langle S_0^z(t)S_R^z(0)\rangle dt, \quad (1)$$

into Lorentzian $S_L'(K,\omega)$ and Gaussian $S_G'(K,\omega)$ parts. These were then assumed[2] to be given by a revised two-parameter representation of the Lorentzian,

$$S_L'(K,\omega)=\left[\frac{S(S+1)}{\omega^2+\Gamma_K^2}\right]\left[\frac{\Gamma_K}{2\tan^{-1}(\omega_C/\Gamma_K)}\right], \quad |\omega|<\omega_C$$
$$=0, \quad |\omega|>\omega_C \quad (2)$$

and a Gram-Charlier (GC) form of the Gaussian,

$$S_G'(K,\omega)=[S(S+1)/(2\pi\sigma^2)^{1/2}]\exp(-\omega^2/2\sigma^2)\times\{1+b_K[\omega^4/\sigma^4-6(\omega^2/\sigma^2)+3]\}. \quad (3)$$

The Lorentzian and Gaussian parts of the spectral function were chosen to conserve separately, in the limit of elevated temperature, the zeroth-moment sum rules,

$$\frac{a}{2\pi}\int_{-\pi/a}^{\pi/a}dK\int_{-\infty}^{\infty}d\omega\, S(K,\omega)=S(S+1), \quad (4)$$

$$\int_{-\infty}^{\infty}S(K,\omega)d\omega=S(S+1), \quad (5)$$

as well as the second and fourth frequency moments. The frequency moments are given by the following:

$$\langle\omega^{2m}\rangle_K=\int_{-\infty}^{\infty}\omega^{2m}S(K,\omega)d\omega\Big/\int_{-\infty}^{\infty}S(K,\omega)d\omega,$$
$$\langle\omega^{2m+1}\rangle_K=0. \quad (6)$$

A suitably weighted linear combination of $S_L'(K,\omega)$ and $S_G'(K,\omega)$ was then formed to construct the spectral function $S(K,\omega)$, i.e.,

$$S(K,\omega)=W_n^+(K)S_L'(K,\omega)+W_n^-(K)S_G'(K,\omega), \quad (7)$$

where the weighting factors are given by

$$W_n^{\pm}(K)=(\gamma_0^{2n+1}\pm\gamma_K^{2n+1})/2\gamma_0^{2n+1} \quad (8)$$

and

$$\gamma_K=2\cos Ka. \quad (9)$$

The frequency–wave-vector Fourier transform of the

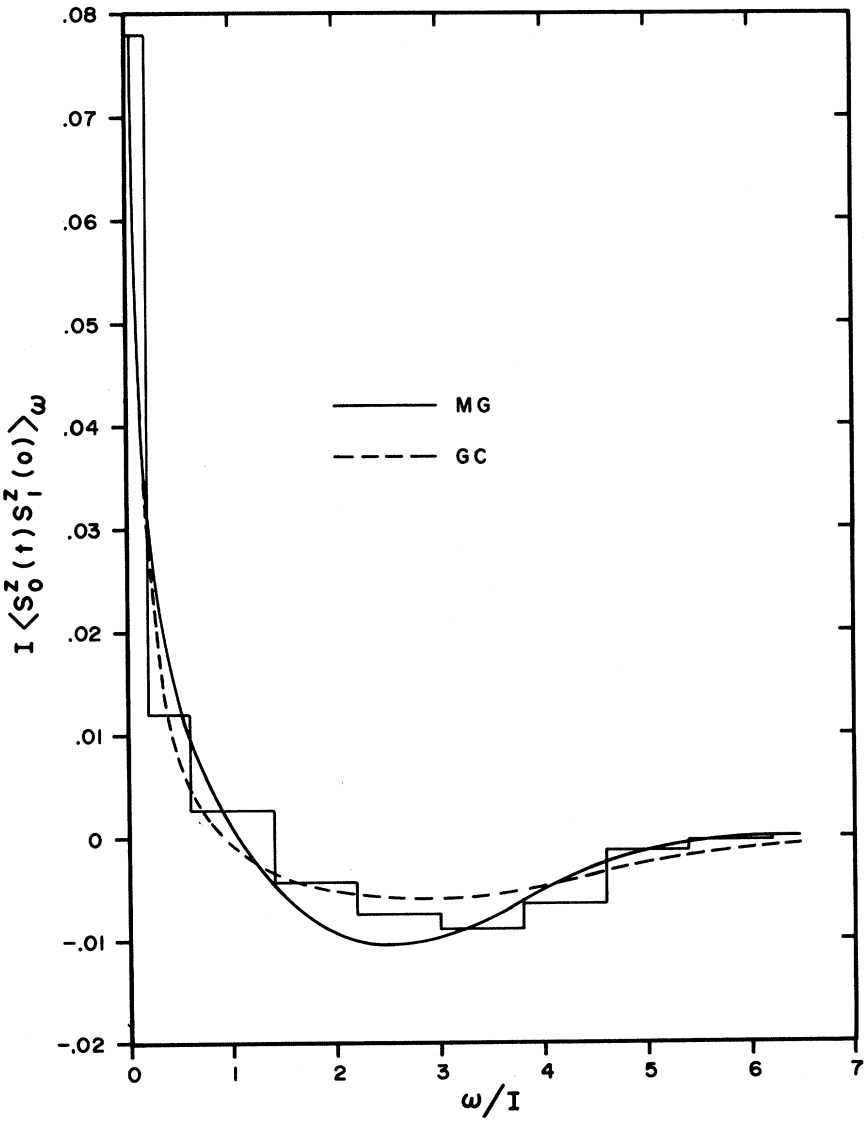

FIG. 3. Comparison of the Fourier transform of the first-nearest-neighbor spin ($S=\frac{1}{2}$) correlations in the MG (full lines) with $n=0$ and the GC (broken lines) against the Carboni-Richard's (CR) results (see Ref. 3) given as histograms.

paramagnetic spin-correlation function is

$$\langle S_0^z(t)\,S_R^z(0)\rangle_\omega = \frac{a}{2\pi}\int_0^{2\pi/a} S(K,\omega)\,\exp(-iK\cdot R)\,dK \tag{10}$$

for a one-dimensional spin system.

The second and fourth frequency moments for a one-dimensional, isotropic Heisenberg spin system (linear chain) at infinite temperature for $S=\frac{1}{2}$ and in the case of a nearest-neighbor approximation are

$$\langle\omega^2\rangle_K = 4I^2(1-\cos Ka),$$
$$\langle\omega^4\rangle_K = 8I^4(1-\cos Ka)(4-3\cos Ka), \tag{11}$$

where I = exchange integral.

The Lorentzian and Gaussian parameters, which are functions of K, are then separately determined by Eq. (6), i.e.,

$$\langle\omega^2\rangle_K = \frac{\omega_C\Gamma_K}{\tan^{-1}(\omega_C/\Gamma_K)} - \Gamma_K^2,$$
$$\langle\omega^4\rangle_K = \frac{\frac{1}{3}(\omega^3\Gamma_K) - \Gamma_K^3\omega_C}{\tan^{-1}(\omega_C/\Gamma_K)} + \Gamma_K^4, \tag{12}$$

and

$$\langle\omega^2\rangle_K = \sigma^2, \qquad \langle\omega^4\rangle_K = 24\sigma^4(b_K+\tfrac{1}{8}). \tag{13}$$

This procedure, however, has two possible weaknesses. First, the choice of the weighting factor $W_n^{\pm}(K)$ for the Lorentzian and Gaussian parts of the spectral function

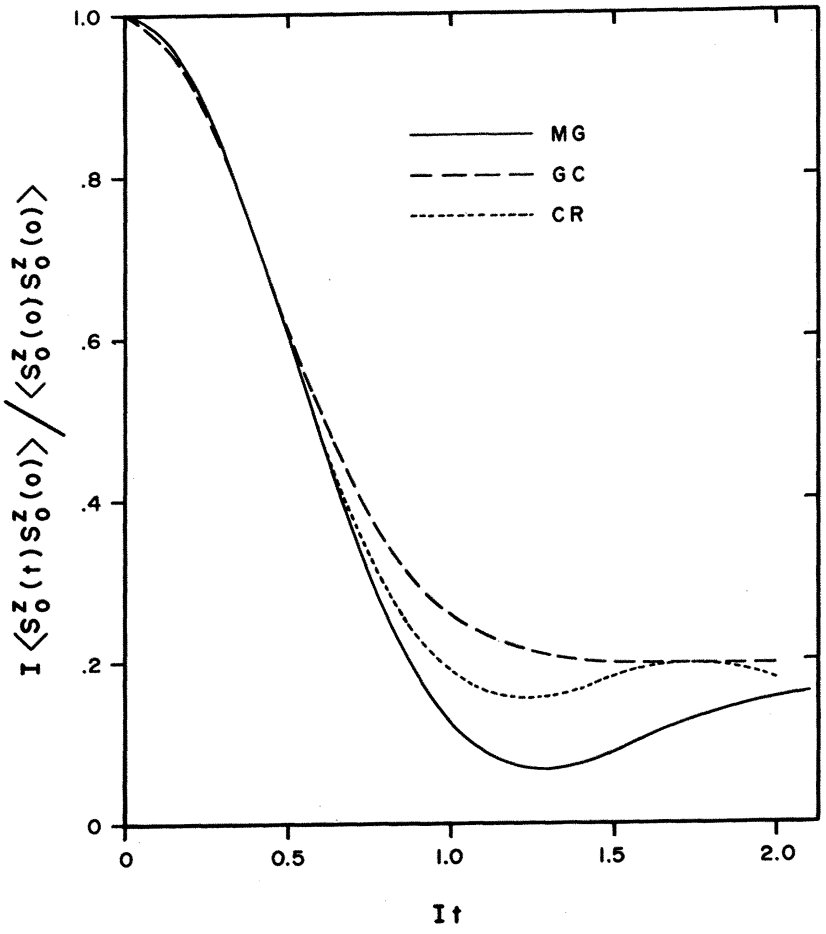

FIG. 4. Time-dependent self-correlation for $S=\frac{1}{2}$, one-dimensional, isotropic Heisenberg ferromagnet at $T=\infty$. The full curve is obtained with the MG and the broken curve with the CG procedure. The CR results lie inbetween these two curves (i.e., dashed line).

$S(K,\omega)$ is subject to a great deal of arbitrariness because the physical requirement of the FG suggestion can be satisfied for any positive integral (or zero) value of the index n. Second, the Gram-Charlier representation of the Gaussian part of the spectral function line shape contains in itself the possibility of leading to a physically unacceptable spectral function, i.e., which may violate the rigorous non-negativity requirement that $S(K,\omega)>0$ for all (positive and negative) values of ω and all allowed values of K.

The object of the present note is first to record the observation that the former of these two possible difficulties is in practice rather innocuous and that most of the final results are relatively insensitive to the magnitude of n (see Figs. 1 and 2). Second, in this paper we report an examination of the adequacy of the GC representation (for the Gaussian part of the FG spectral function line shape) given in Eq. (3), which as remarked earlier, can violate the rigorous non-negativity requirement, against the modified Gaussian form (MG) proposed in Ref. 2, i.e.,

$$S_G'(K,\omega)=A^2(K)\exp[-B^2(K)\omega^2][1+C^2(K)\omega^2], \tag{14}$$

which does not violate this requirement. The coefficients $A(K)$, $B(K)$, and $C(K)$ are determined by Eq. (6), i.e.,

$$\begin{aligned} 1&=\sqrt{\pi}[A^2(K)/B(K)][1+C^2(K)/2B^2(K)], \\ \langle\omega^2\rangle_K&=(\sqrt{\pi}/2)[A^2(K)/B^3(K)] \\ &\quad\times[1+3C^2(K)/2B^2(K)], \\ \langle\omega^4\rangle_K&=(3\sqrt{\pi}/4)[A^2(K)/B^5(K)] \\ &\quad\times[1+5C^2(K)/2B^2(K)]. \end{aligned} \tag{15}$$

We find that the resultant line shapes obtained by using these two procedures are either very similar (see

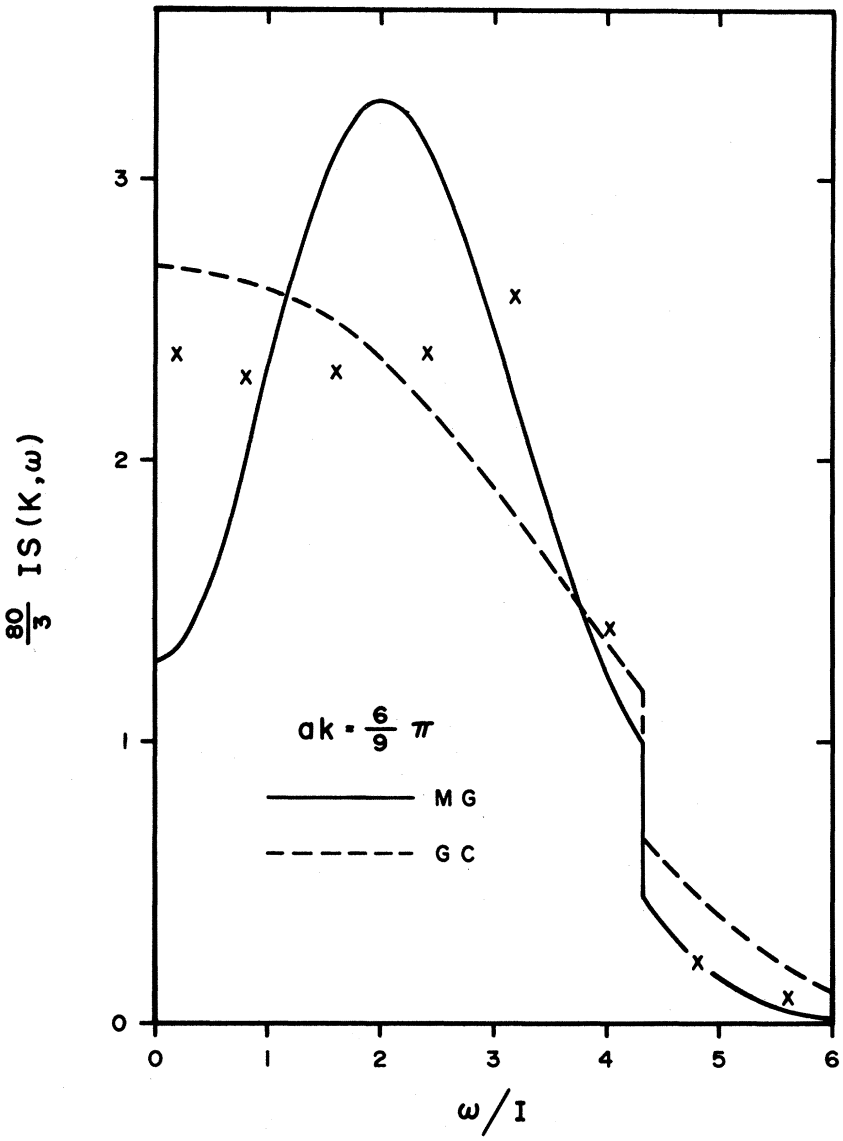

FIG. 5. Comparison of the MG and the GC results for the spin($S=\frac{1}{2}$) spectral function $S(K, \omega)$ for an isotropic Heisenberg linear chain in the limit of elevated temperatures.

Fig. 3), or when they appreciably differ from each other (see Figs. 4 and 5), then they do so in a way that neither of them is a particularly good representation of the actual line shape (see, for example, Fig. 5, where the rather reliable results of the Carboni-Richards[3] computation, shown as crosses, are poorly represented by the MG and GC curves).

We are greatly indebted to the Temple University Computer Center for the use of their Computer CDC-6400.

* Supported by a Long Term Training Grant, Department of the U.S. Army.
† Supported by the Office of Naval Research.

[1] J. F. Fernandez and H. A. Gersch, Phys. Rev. **172**, 341 (1968).

[2] D. G. McFadden, R. A. Tahir-Kheli, and G. B. Taggart, Phys. Rev. **185**, 854 (1969). (The notation of this reference is used throughout this paper.)

[3] F. Carboni and P. M. Richards, Phys. Rev. **177**, 889 (1969).