Short Notes

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A Fundamental Breakdown of an Approximation to the Heisenberg Ferromagnet

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The low temperature magnetization of a Heisenberg ferromagnet was calculated by Dyson /1/ with the help of ideal spin wave (Bose) operators to contain a T^4 term but no T^3 term. This result could not yet be reproduced satisfactorily using spin operator Green functions (GF) /2/. To take into account the algebraic properties of the spin operator GF and to improve the results more complicated decoupling schemes were proposed by Callen /3/, Dembiński /4/, and many other authors /5/.

Dembiński's decoupling /4/ yields a T^4 term but no T^3 term in the low temperature magnetization. However, up to now the energy of the spin waves resulting from the GF after Dembiński's decoupling is not known. It is the aim of this short note to calculate the spectral density for the GF after Dembiński's decoupling for a linear chain and a three-dimensional simple cubic lattice. The result will be that Dembiński's approximation violates the positivity of the spectral density.

An exact solution of the equations of motion for the GF after Dembiński's decoupling was given by Englisch et al. /6/ and independently by Tenan and Ramos /7/. The solutions found in /6/ and /7/ are identical. The analytic properties of this exact solution for finite N were discussed in /6/, while some special cases were investigated in /7/.

We are now going to calculate the GF for a linear chain in the continuous limit $N \to \infty$. The only approximation involved is Dembiński's decoupling. The exact solution of the equations of motion after Dembiński's decoupling is /6/

$$G(E, \vec{k}) = \frac{i\sigma}{2\pi} \frac{1}{E - \Omega_{\vec{k}}} \left(1 + \frac{A\omega_{\vec{k}} \sum_{\vec{q}} \frac{\gamma_{\vec{q}}}{E - \Omega_{\vec{q}}}}{1 - A \sum_{\vec{q}} \frac{\gamma_{\vec{q}}\, \omega_{\vec{q}}}{E - \Omega_{\vec{q}}}} \right) \tag{1}$$

with the notations

$$A = \sigma\, (\sigma - 1)J/(N\gamma_0)\ , \qquad \gamma_{\vec{k}} = \sum_{\vec{\delta}} e^{i\vec{\delta}\vec{k}}\ , \qquad \omega_{\vec{k}} = \gamma_0 - \gamma_{\vec{k}}\ ,$$

$$\Omega_{\vec{k}} = 2R\,\omega_{\vec{k}}\ , \qquad R = 1 + \frac{2}{N} \sum_{\vec{q}} \frac{\gamma_{\vec{q}}}{\gamma_0}\, \Psi(\vec{q})\ , \qquad \sigma = \langle S_f^z \rangle .$$

$\Psi(\vec{q})$ is the Fourier transform of the correlation function $\langle S_f^+ S_g^- \rangle$. For the special case of a continuous linear chain we have $\gamma_q = 2\cos aq$, where $-\pi/a \leqq q \leqq \pi/a$. Omitting the straight-forward calculations we write down the resulting GF for the linear chain

$$G(E, k) = \frac{i\sigma}{2\pi} \frac{1}{(E - \Omega_k)\, [1 + Ef(E)]} + \frac{i\sigma}{2\pi} \frac{f(E)}{1 + Ef(E)}\ , \tag{2}$$

where

$$f(E) = \frac{\pm\, iA(2R - E)}{R^2 \sqrt{E(4R - E)}} - \frac{A}{R^2}\ . \tag{3}$$

The upper sign in (3) belongs to the upper edge of the cut from 0 to 4R in the complex E plane, the minus sign refers to the lower edge. The discontinuity of f(E) arises from the integration across the poles $E = \Omega_q$.

The first term of the GF (2) looks like a simple pole at $E = \Omega_k$ modified by a factor which gives rise to a cut from E = 0 to E = 4R along the real axis. From the very beginning, the second term is an unusual one, since there is no dependence on k in it; it has a cut from E = 0 to E = 4R along the real axis, too.

The spectral density is defined by the Hilbert transformation

$$G(E, \vec{k}) = \frac{i}{2\pi} \int \frac{\varrho(\omega, \vec{k})\, d\omega}{\omega - E + i\varepsilon}\ ; \tag{4}$$

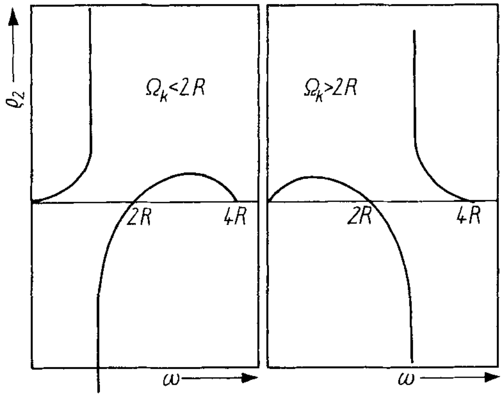

Fig. 1. Second term of the spectral density (5)

$\varrho(\omega, \vec{k})$ is calculated from $\varrho(\omega, \vec{k}) = G(\omega + i\varepsilon, \vec{k}) - G(\omega - i\varepsilon, \vec{k})$ in the limit $\varepsilon \to 0$. We start with the first term in (2) writing it in the form $i\sigma/(2\pi)(a \pm ib)/(E - \Omega_k)$ and obtain

$$G(\omega + i\varepsilon, k) - G(\omega - i\varepsilon, k) = \frac{i\sigma}{2\pi}\left[\frac{a + ib}{\omega - \Omega_k + i\varepsilon} - \frac{a - ib}{\omega - \Omega_k - i\varepsilon}\right],$$

where we used the relation $\lim_{\varepsilon \to 0} \frac{1}{x \pm i\varepsilon} = P\frac{1}{x} \mp i\pi\delta(x)$. The discontinuity of the second term in (2) is

$$-\frac{\sigma}{\pi} \,\mathrm{Im}\left(\frac{f(E)}{1 + Ef(E)}\right).$$

The explicit expression for $\varrho(\omega, k)$ is

$$\varrho(\omega, k) = \frac{1}{D}\left[\left(1 - \frac{A\omega}{R}\right)\delta(\omega - \Omega_k) - \frac{\sigma A \omega(2R - \omega)}{\pi R^2 \sqrt{\omega(4R - \omega)}} P\frac{1}{\omega - \Omega_k} + \right.$$

$$\left. + \frac{A(2R - \omega)}{R^2\sqrt{\omega(4R - \omega)}}\right], \tag{5}$$

where

$$D = 1 - \frac{2A\omega}{R} + \frac{A^2\omega^2}{R^2} + \frac{A^2\omega(2R - \omega)^2}{4R - \omega}. \tag{6}$$

If we look at the local properties of the distribution $P\frac{1}{x}$ we get the curves shown in Fig. 1 and 2 for the second and the third term of (5), respectively.

From Fig. 1 and 2 we see that $\varrho(\omega, k)$ is not non-negative, as it should be from general considerations /8/. Furthermore, the spectral density (5) does not allow the usual physical interpretation as a (damped) spin wave excitation with possible bound states.

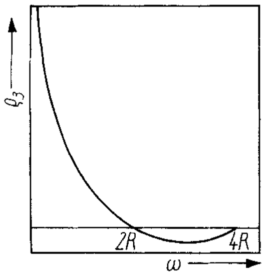

Fig. 2. Third term of the spectral density (5)

We want to emphasize once more that no further approximation has been done after Dembiński's decoupling. On this base we can conclude that Dembiński's decoupling violates fundamental properties of the GF in the one-dimensional case. In particular, there is no interpretation as a spin wave; the first term of ϱ in (5) would allow for an interpretation as an undamped spin wave, however, the change of sign in the second and the third term in (5) makes impossible any physical interpretation.

The contradiction against the requirement of a non-negative spectral density is not restricted to the one-dimensional case. We can show the same contradiction for a three-dimensional simple cubic lattice, too. For a simple cubic lattice we have $\gamma_{\vec{q}} = 2(\cos q_x a + \cos q_y a + \cos q_z a)$ and we have to calculate the integral

$$\iiint dq_x dq_y dq_z \, \frac{(\cos q_x a + \cos q_y a + \cos q_z a)(3 - \cos q_x a - \cos q_y a - \cos q_z a)}{E - 2R(3 - \cos q_x a - \cos q_y a - \cos q_z a)} \qquad (7)$$

among others, which may be obtained from (7), too. In (7) we substitute the variables similar to the one-dimensional case

$$E - 2R(3 - \cos q_x a - \cos q_y a - \cos q_z a) = x \; ,$$

$$1 - \cos q_y a = y, \qquad 1 - \cos q_z a = z \; ,$$

and obtain an expression quite similar to (2) and (3). The essential dependence on E is exactly the same for the GF in the three-dimensional case as in the one-dimensional case. The cut along the real axis is situated from $E = 0$ to $E = 12R$. However, the coefficients in f(E) are no longer as simple as in (3), they are now integrals over elliptic integrals. We do not write down the comparatively complicated expressions, since the conclusions are the same as in the simpler one-dimensional case, and Fig. 1 and 2 remain valid qualitatively.

Very recently, Balakrishnan and Balakrishnan /9/ proposed a decoupling very similar to Dembiński's decoupling, and they solved their equations of motion by successive approximation, too. Therefore, Balakrishnan's approximation also suffers from the same violation for the non-negativity of the spectral density as Dembiński's scheme.

Singer /10/ investigated the compensation of the T^3 term in the low temperature magnetization very carefully and showed that the compensation in Dembiński's approach is exact, what is not the case in other approaches. Nevertheless, Dembiński's decoupling is an example of an approximation scheme giving an improved result for one quantity - the low temperature magnetization - but violating fundamental properties of the calculated GF - the non-negativity of the spectral density.

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