

Low-Temperature Magnetization of the $S = \frac{1}{2}$ Heisenberg Ferromagnet

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The low-temperature magnetization of the $S = \frac{1}{2}$ Heisenberg ferromagnet has been investigated by the method of double-time temperature-dependent Green functions. The equation for the lowest order Green function and the equation for the next higher order Green function, truncated to order $\langle n \rangle = \frac{1}{2} - \langle S^z \rangle$, were solved. The low-temperature magnetization so obtained was found to agree with that obtained by Dyson. In particular, an argument is presented which suggests that the T^3 term, which has previously plagued this method, does indeed vanish.

THE magnetization of a Heisenberg ferromagnet in the low-temperature region has been rigorously studied by Dyson¹ using the method of spin waves. More recently various authors have applied the method of double-time temperature-dependent Green functions to this problem.²⁻⁸ In the case $S = \frac{1}{2}$ there is a discrepancy of order T^3 in the magnetization which arises from an error in the decoupling approximation used to solve the Green-function equation of motion. Tanaka and Morita⁹ have reported the elimination of the T^3 term by solving the equation of motion for the higher order Green function. While their final result appears to be correct, we feel that they did not make the correct approximations in deriving their equation of motion, and hence lost some insight into the results.

Expressing the spin operators of the f th site by the Pauli operators

$$\begin{aligned} S_f^x + iS_f^y &= S_f^+ = b_f, \\ S_f^z &= \frac{1}{2} - b_f^\dagger b_f = \frac{1}{2} - n_f, \end{aligned} \quad (1)$$

satisfying the anticommutation relations

$$\{b_f, b_f^\dagger\} = 1; \quad \{b_f, b_f\} = \{b_f^\dagger, b_f^\dagger\} = 0,$$

and the commutation relations

$$\begin{aligned} [b_f, b_g^\dagger] &= \delta_{gf}(1 - 2n_f); \\ [b_f, n_g] &= \delta_{gf}b_f; \quad [b_f^\dagger, n_g] = -\delta_{gf}b_f^\dagger, \end{aligned} \quad (2)$$

and defining an exchange sum

$$J(\mathbf{k}) = \sum_f e^{i\mathbf{k}\cdot(\mathbf{f}-\mathbf{m})} I(\mathbf{f}-\mathbf{m}), \quad \text{where } I(0) = 0, \quad (3)$$

the Heisenberg exchange Hamiltonian with an external field H becomes

$$\begin{aligned} \mathcal{H} &= [\mu H + \frac{1}{2}J(0)] \sum_f n_f \\ &\quad - \frac{1}{2} \sum_{f,m} I(\mathbf{f}-\mathbf{m})(b_f^\dagger b_m + n_f n_m). \end{aligned} \quad (4)$$

We will consider the two Green functions $G_{gf} = \langle\langle b_g; b_{gf} \rangle\rangle$ and $G_{glmf} = \langle\langle b_g^\dagger b_l b_m; b_f^\dagger \rangle\rangle$. The departure of the magnetization from saturation is then given by

$$\langle n \rangle = \frac{1}{N} \sum_g i \int_{-\infty}^{\infty} \frac{[G_{gg}(E+i\epsilon) - G_{gg}(E-i\epsilon)]}{e^{\beta E} - 1} dE. \quad (5)$$

The reader is referred to Zubarev³ for details of the Green-function method.

The Green functions are determined from their equations of motion:

$$\begin{aligned} [E - \mu H - \frac{1}{2}J(0)]G_{gf} &= -\frac{1}{2\pi} \delta_{gf} \langle 1 - 2n_f \rangle - \frac{1}{2} \sum_m I(\mathbf{g}-\mathbf{m})G_{mf} \\ &\quad + \sum_m I(\mathbf{g}-\mathbf{m})[G_{gqm} - G_{mmq}] \end{aligned} \quad (6)$$

and

$$\begin{aligned} [E - \mu H - \frac{1}{2}J(0)]G_{glmf} &= (1/2\pi) \delta_{lf} \langle b_g^\dagger b_m - 2b_g^\dagger n_f b_m \rangle \\ &\quad + (1/2\pi) \delta_{mj} \langle b_g^\dagger b_l - 2b_g^\dagger n_l b_j \rangle \\ &\quad + \frac{1}{2} \sum_p I(\mathbf{g}-\mathbf{p})G_{plmf} - \frac{1}{2} \sum_p I(\mathbf{m}-\mathbf{p})G_{plpf} \\ &\quad - \frac{1}{2} \sum_p I(\mathbf{l}-\mathbf{p})G_{pmpf} \\ &\quad + \frac{1}{2} \sum_p I(\mathbf{g}-\mathbf{p}) \langle\langle b_g^\dagger b_l b_m n_p + n_p b_g^\dagger b_l b_m \\ &\quad \quad - 2b_p^\dagger n_g b_l b_m; b_f^\dagger \rangle\rangle \\ &\quad - \frac{1}{2} \sum_p I(\mathbf{m}-\mathbf{p}) \langle\langle b_g^\dagger b_l b_m n_p + n_p b_g^\dagger b_l b_m \\ &\quad \quad - 2b_g^\dagger b_l n_m b_p; b_f^\dagger \rangle\rangle \\ &\quad - \frac{1}{2} \sum_p I(\mathbf{l}-\mathbf{p}) \langle\langle b_g^\dagger b_l b_m n_p + n_p b_g^\dagger b_l b_m \\ &\quad \quad - 2b_g^\dagger n_l b_m b_p; b_f^\dagger \rangle\rangle. \end{aligned} \quad (7)$$

At this stage we must make some decoupling approximation in Eq. (7). We notice that G_{gf} has a leading term of order 1 and a next higher term of order $\langle n \rangle$ which is small at low temperatures. The function G_{glmf} has a leading term of order $\langle n \rangle$ and higher terms which are of

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⁶ T. Oguchi and A. Honma, J. Appl. Phys. **34**, 1153 (1963).
⁷ R. A. Tahir-Kheli, Phys. Rev. **132**, 689 (1963).
⁸ C. Warren Haas and H. S. Jarrett, Central Research Department Report No. 953, E. I. du Pont de Nemours and Company (unpublished).
⁹ T. Tanaka and T. Morita, Bull. Am. Phys. Soc. **9**, 463 (1964).

order $\langle n \rangle^2$ except for certain values of the indices. We rewrite Eq. (7) keeping only the lowest order terms. Consider for example $\langle b_g^\dagger b_f^\dagger b_f b_m \rangle$. If $f=m$ or $f=g$ this term is zero, otherwise it is of order $\langle n \rangle^2$. However, $\langle b_g^\dagger b_i b_f^\dagger b_f \rangle = \langle b_g^\dagger b_f^\dagger b_f b_i \rangle + \delta_{if} \langle b_g^\dagger b_i \rangle$, so we keep the $\delta_{if} \langle b_g^\dagger b_i \rangle$. This is where we differ from Tanaka and Morita who dropped all the products of four operators without regard to their order. They partially compensate for this error by carrying a subsidiary condition along, namely $G_{gilmf} = 0$ if $l=m$.

After a similar analysis of the last three sums in Eq. (7) we are left with an approximate equation of motion

$$\begin{aligned} [E - \mu H - \frac{1}{2}J(0)]G_{gilmf} &= (1/2\pi)\delta_{if}\langle b_g^\dagger b_m \rangle + (1/2\pi)\delta_{mf}\langle b_g^\dagger b_i \rangle \\ &\quad - (2/2\pi)\delta_{mf}\delta_{if}\langle b_g^\dagger b_i \rangle + \frac{1}{2}\sum_p I(\mathbf{g}-\mathbf{p})G_{plmf} \\ &\quad - \frac{1}{2}\sum_p I(\mathbf{m}-\mathbf{p})G_{gipf} - \frac{1}{2}\sum_p I(\mathbf{l}-\mathbf{p})G_{gpmf} \\ &\quad - I(\mathbf{m}-\mathbf{l})G_{gilmf} + \delta_{ml}\sum_p I(\mathbf{m}-\mathbf{p})G_{gipf}. \quad (8) \end{aligned}$$

The equation of Tanaka and Morita is identical except for the absence of the third and eighth terms on the right-hand side of Eq. (8). However, their approximate solution is exactly what we would obtain by dropping the seventh and eighth terms in our Eq. (8) but retaining the third, $-(2/2\pi)\delta_{mf}\delta_{if}\langle b_g^\dagger b_i \rangle$. The effect of our third term appears in Tanaka and Morita's solution through their subsidiary condition. Notice that Eq. (8) automatically gives $G_{gulf} = 0$.

The solution is most easily found by expanding G_{gf} and G_{gilmf} in reciprocal lattice vectors:

$$\begin{aligned} G_{gf} &= \frac{1}{N} \sum_{\lambda} \exp[i\lambda \cdot (\mathbf{g}-\mathbf{f})] G_{\lambda}, \\ G_{gilmf} &= \frac{1}{N^3} \sum_{\lambda\lambda'\lambda''} \exp[i\lambda \cdot (\mathbf{g}-\mathbf{f})] \exp[i\lambda' \cdot (\mathbf{l}-\mathbf{f})] \\ &\quad \times \exp[i\lambda'' \cdot (\mathbf{m}-\mathbf{f})] G_{\lambda\lambda'\lambda''}, \quad (9) \end{aligned}$$

$$\begin{aligned} \langle b_g^\dagger b_f \rangle &= \frac{1}{N} \sum_{\lambda} \exp[i\lambda \cdot (\mathbf{g}-\mathbf{f})] n_{\lambda}, \\ n_{\lambda} &= i \int_{-\infty}^{\infty} \frac{G_{\lambda}(E+i\epsilon) - G_{\lambda}(E-i\epsilon)}{e^{\beta E} - 1} dE, \end{aligned}$$

$$E(\lambda) = \mu H + \frac{1}{2}[J(0) - J(\lambda)].$$

The equations of motion become

$$\begin{aligned} [E - E(\lambda)]G_{\lambda} &= \frac{1 - \langle n \rangle}{2\pi} \\ &\quad + \frac{1}{N^2} \sum_{\nu\nu'} [J(\lambda - \nu - \nu') - J(\nu + \nu')] G_{\nu\nu'\lambda - \nu - \nu'}, \quad (10) \end{aligned}$$

$$[E - E(\lambda') - E(\lambda'') + E(\lambda)]G_{\lambda\lambda'\lambda''}$$

$$= -\frac{N}{2\pi} [\delta(\lambda + \lambda') + \delta(\lambda + \lambda'')] n_{\lambda}$$

$$- \frac{2n_{\lambda}}{2\pi} - \frac{1}{N} \sum_k [E(\lambda'' + \mathbf{k})$$

$$+ E(\lambda' - \mathbf{k}) - 2E(\mathbf{k})] G_{\lambda\lambda' - \mathbf{k}\lambda'' + \mathbf{k}}. \quad (11)$$

If we solve Eq. (11) approximately by dropping the sum over \mathbf{k} we have

$$G_{\lambda\lambda'\lambda''} \approx \frac{N[\delta(\lambda + \lambda') + \delta(\lambda + \lambda'')] - 2}{2\pi[E - E(\lambda') - E(\lambda'') + E(\lambda)]} n_{\lambda} \quad (12)$$

and

$$[E - E(\lambda)]G_{\lambda} = \frac{1 - 2\langle n \rangle}{2\pi}$$

$$+ \frac{1}{N} \sum_{\nu} \frac{J(\lambda) - J(0) + J(\nu) - J(\lambda + \nu)}{2\pi[E - E(\lambda)]} n_{\nu}$$

$$- \frac{1}{N^2} \sum_{\nu\nu'} \frac{J(\lambda - \nu - \nu') - J(\nu + \nu')}{2\pi[E - E(\nu') - E(\lambda - \nu - \nu') + E(\nu)]} 2n_{\nu}. \quad (13)$$

After substituting this result into Eq. (5) we find that the second term on the right side of Eq. (13) is the correct energy renormalization which affects $\langle n \rangle$ to order T^4 . We have shown¹⁰ that the third term on the right cancels the contribution of the $-2\langle n \rangle/2\pi$ in the first term through order T^3 , in agreement with Tanaka and Morita. The problem remaining is to investigate the effect of the last term in Eq. (11), that is, the sum over \mathbf{k} . We have iterated this equation twice, substituted the results into Eq. (5), and found no contribution larger than T^4 . It seems possible that the iterations are convergent in this sense but a definite proof is still lacking.

It should be pointed out that $G_{\lambda\lambda'\lambda''}$ does give $\langle b_g^\dagger b_g^\dagger b_i b_m \rangle = 0$ but does not give $\langle b_f^\dagger b_g^\dagger b_i b_i \rangle = 0$. For that we must include the effect of the eighth term of Eq. (8). It can be shown that inclusion of the first iteration of Eq. (11) gives $\langle b_f^\dagger b_g^\dagger b_i b_i \rangle = 0$ through order T^3 or $\langle n \rangle^2$, although as we have said it does not contribute to $\langle n \rangle$ until order T^4 . This can be explained by the fact that terms such as G_{gggf} are excluded completely from the sum in Eq. (6) and hence do not need to be known exactly, while G_{ggmg} does contribute and must be known.

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¹⁰ I. Ortenburger, Doctoral dissertation, Stanford University, 1964 (unpublished).