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Comment on a mean-field theory of quantum antiferromagnets

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We show that the mean-field theory of quantum Heisenberg models introduced by Arovas and Auerbach predicts long-range order for all dimensions $d \gtrsim 2$ in the ground state as well as below a critical temperature $T_c(d)$ that is nonzero for $d>2$. The long-range order in the ground state is the same as predicted by conventional spin-wave theory.

Functional integral theories of quantum Heisenberg models were recently discussed by Arovas and Auerbach (AA).[1] For dimensions larger than 1 they found that a boson mean-field theory yields a lower free energy than a fermion mean-field theory and, thus, they suggest that the former one is valid. They focus their discussion on the disordered state at finite temperatures and show that below a temperature $T_- > 0$ for $d>2$ no solution of the mean-field equations for the disordered state exists. Thus, they suggest that T_- should be associated with the Néel temperature.

In this Comment, we point out that the AA theory in fact predicts long-range order below a critical temperature in dimensions greater than 2, as well as in the ground state for dimensions equal to 2. Our reasoning closely parallels the well-known analysis of Bose-Einstein condensation:[2] Below a critical temperature, passage from a sum to an integral becomes invalid as one (or in this case two) terms contribute a finite fraction to the total sum. The long-range order obtained in the ground state in the thermodynamic limit is the same as the one predicted by Anderson's spin-wave theory.[3,4]

The spin-spin correlation function for a quantum antiferromagnet on an N-site lattice is given within AA's mean-field theory by

$$\langle \mathbf{S}_0 \cdot \mathbf{S}_R \rangle = (|f(R)|^2 - |g(R)|^2) - \tfrac{1}{4}\delta_{R,0}, \tag{1}$$

where

$$f(R) = \frac{1}{2N}\sum_k e^{i\mathbf{k}\cdot\mathbf{R}} \frac{\coth(\beta\omega_k/2)}{(1-\eta^2\gamma_k^2)^{1/2}}, \tag{2a}$$

and

$$g(R) = \frac{1}{2N}\sum_k e^{i\mathbf{k}\cdot\mathbf{R}} \frac{\eta\gamma_k \coth(\beta\omega_k/2)}{(1-\eta^2\gamma_k^2)^{1/2}}, \tag{2b}$$

with

$$\gamma_k = \frac{1}{d}\sum_{\nu=1}^{d} \cos k_\nu, \tag{3a}$$

and

$$\omega_k = c\sqrt{2(1-\eta^2\gamma_k^2)}. \tag{3b}$$

The parameter $\eta \leq 1$ and spin-wave velocity c are determined by the constraint equations[1]

$$2S+1 = \frac{1}{N}\sum_k \frac{\coth(\beta\omega_k/2)}{(1-\eta^2\gamma_k^2)^{1/2}}, \tag{4a}$$

$$c = \frac{\sqrt{2}}{N}\sum_k \frac{\gamma_k^2 \coth(\beta\omega_k/2)}{(1-\eta^2\gamma_k^2)^{1/2}}. \tag{4b}$$

We have included in Eq. (1) a normalization factor $\frac{2}{3}$ so that the condition $\langle \mathbf{S}_0 \cdot \mathbf{S}_R \rangle = S(S+1)$ is satisfied, as suggested by AA.[1] The structure factor at wave vector $\boldsymbol{\pi}$ is given by

$$S(\boldsymbol{\pi}) = \sum_R (-1)^R \langle \mathbf{S}_0 \cdot \mathbf{S}_R \rangle = \left(\frac{1}{4N}\right)\sum_k \frac{1+\eta^2\gamma_k^2}{1-\eta^2\gamma_k^2}\coth^2\left(\frac{\beta\omega_k}{2}\right) - \frac{1}{4}, \tag{5}$$

and in the thermodynamic limit it is related to the mean-squared staggered magnetization m by

$$Nm^2 = S(\boldsymbol{\pi}), \tag{6}$$

where the order parameter $m^2 = \langle [\sum_k (-1)^R \mathbf{S}_R]^2 \rangle$.

We now use the above equations to calculate the ground-state magnetization in the thermodynamic limit. *First* we take the limit $T \rightarrow 0$ on a finite lattice and then let $N \rightarrow \infty$. As $T \rightarrow 0$, Eqs. (4a) and (4b) will be decoupled; only Eq. (4a) is needed to determine η, and the spin-spin correlations do not depend on the value of the spin-wave velocity c.

As $T \to 0$, Eq. (4a) simply becomes

$$2S+1=\frac{1}{N}\sum_k \frac{1}{(1-\eta^2\gamma_k^2)^{1/2}} . \tag{7}$$

As pointed out by AA, the right-hand side of Eq. (7) is an increasing function of η. The integral that one obtains from the right-hand side of Eq. (7) in the limit $N \to \infty$,

$$I=\int \frac{d^dk}{(2\pi)^d}\frac{1}{(1-\eta^2\gamma_k^2)^{1/2}} , \tag{8}$$

is nondivergent in $d>1$, and as $\eta \to 1$ takes the values $I=1.3932$ and $I=1.156$ (Ref. 3) for $d=2$ and $d=3$, respectively. Thus, it would appear that Eq. (7) cannot be satisfied for any $S \geq \frac{1}{2}$. However, passage from the sum to the integral will be invalid as $\eta \to 1$. Following the analogous treatment for Bose-Einstein condensation,[2] we separate the divergent terms at $\mathbf{k}=\mathbf{0}$ and $\mathbf{k}=\boldsymbol{\pi}$ from the sum to yield

$$2S+1=\frac{2}{N(1-\eta^2)^{1/2}}+\int \frac{d^dk}{(2\pi)^d}\frac{1}{(1-\eta^2\gamma_k^2)^{1/2}} , \tag{9}$$

which can be satisfied by an η that differs from unity by $O(1/N^2)$. The value of η is easily obtained from Eq. (9) by setting $\eta=1$ inside the integral. It is easy to convince oneself, following analogous arguments for Bose-Einstein condensation, that no other $\mathbf{k}$ values contribute a finite fraction to the sum in Eq. (7) for large N.

The long-range order can now be obtained from Eq. (6) as

$$Nm^2=\frac{1}{2N}\frac{1+\eta^2}{1-\eta^2}+\frac{1}{4}\int \frac{d^dk}{(2\pi)^d}\frac{1+\gamma_k^2}{1-\gamma_k^2}-\frac{1}{4} . \tag{10}$$

Because the integral Eq. (10) is nondivergent at $d=3$ and diverges only as $\ln N$ at $d=2$, it gives no contribution to the long-range order in the thermodynamic limit in either case, and the long-range order is given by

$$m=\frac{1}{N}\frac{1}{(1-\eta^2)^{1/2}} . \tag{11}$$

We have, then, from Eq. (9)

$$m=\frac{1}{2}\left[2S+1-\int \frac{d^dk}{(2\pi)^d}\frac{1}{(1-\gamma_k^2)^{1/2}}\right] , \tag{12}$$

which is identical to Anderson's[3] expression from spin-wave theory, yielding for $S=\frac{1}{2}$ a long-range order $m=0.303$ and $m=0.422$ in $d=2$ and $d=3$, respectively.

At finite-temperatures, the summation in Eq. (4a) diverges in two dimensions in the thermodynamic limit if $\eta=1$. Equation (4a) can, therefore, be satisfied at any finite temperature with $\eta<1$, yielding a finite value for $S(\pi,\pi)$ and no long-range order. Thus, there is no phase transition at finite temperature in $d=2$ in agreement with what one would expect from the Mermin-Wagner theorem.[5] In three dimensions, the right-hand side of Eq. (4a) is nondivergent. We can find the critical temperature T_c by setting $\eta=1$ in Eq. (4a), solving (4a) for (βc), and (4b) for c. We find for $S=\frac{1}{2}$ $T_c=4.30$ to be compared with high-temperature series estimates $T_c \sim 3.83$.[6] For $T<T_c$, we have

$$\frac{1}{N}\frac{1}{(1-\eta^2)^{1/2}}=\frac{1}{2}\left[2S+1-\int \frac{d^dk}{(2\pi)^d}\frac{\coth(\beta\omega_k/2)}{(1-\gamma_k^2)^{1/2}}\right] , \tag{13a}$$

$$c=\frac{\sqrt{2}}{N}\frac{1}{(1-\eta^2)^{1/2}}+\frac{\sqrt{2}}{N}\int d^dk\, \frac{\gamma_k^2\coth(\beta\omega_k/2)}{(1-\gamma_k^2)^{1/2}} , \tag{13b}$$

to be solved self-consistently for c and η, and m is obtained from Eq. (11).

In summary, we have shown that the mean-field theory of quantum antiferromagnets introduced by Arovas and Auerbach yields sensible predictions for the ordered phase of quantum antiferromagnets in dimensions $d=2$ and greater. The equations have a solution with finite long-range order for dimensions $d \geq 2$ at $T=0$, and for $T<T_c$ for $d>2$, analogous to the case of Bose-Einstein condensation. The long-range order in the ground state coincides with that obtained from Anderson's spin-wave theory.

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[1]D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988); A. Auerbach and D. P. Arovas, Phys. Rev. Lett. **61**, 617 (1988).

[2]See, for example, K. Huang, *Statistical Mechanics* (McGraw-Hill, New York, 1956), Chap. 12.

[3]P. W. Anderson, Phys. Rev. **86**, 694 (1952).

[4]We are grateful to D. Arovas for correcting an incorrect statement on this point in an earlier version of this paper.

[5]N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[6]G. S. Rushbrook, G. A. Baker, and P. J. Wood, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. Green (Academic, New York, 1974), Vol. III, p. 245.