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Abstract

It is shown how the propagator formalism can be used to obtain the low-temperature expansion of the free energy of an isotropic Heisenberg antiferromagnet. The lowest-order terms in such an expansion can be calculated using the proper self-energy evaluated at zero temperature. The analytic properties of this quantity are investigated by expressing it in terms of time ordered diagrams. The low-temperature expansion of the free energy is shown to be of the form $AT^4+BT^4+CT^8$, where *A, B*, and *C* are given by Oguchi correctly to order $1/S$. For spin ½ the term in $1/S^2$ gives a 2% reduction in *A* for a body-centered lattice.

Disciplines

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Comments

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Low-Temperature Properties of a Heisenberg Antiferromagnet*

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It is shown how the propagator formalism can be used to obtain the low-temperature expansion of the free energy of an isotropic Heisenberg antiferromagnet. The lowest-order terms in such an expansion can be calculated using the proper self-energy evaluated at zero temperature. The analytic properties of this quantity are investigated by expressing it in terms of time ordered diagrams. The low-temperature expansion of the free energy is shown to be of the form $AT^4+BT^6+CT^8$, where A, B, and C are given by Oguchi correctly to order $1/S$. For spin $\frac{1}{2}$ the term in $1/S^2$ gives a 2% reduction in A for a body-centered lattice.

THE low-temperature properties of magnetic systems governed by a Heisenberg Hamiltonian have been intensively studied. For the ferromagnet, Dyson[1] has shown how to obtain the virial series by systematic use of perturbation theory. More recently attempts have been made to reproduce his results using Green's function methods. These calculations have not been altogether satisfactory because: (a) there is some ambiguity in the decoupling procedure, and (b) it is difficult to obtain the low-temperature expansion of the free energy by isolating terms with a given temperature dependence. For ferrimagnets and antiferromagnets the progress has been less substantial, as Dyson's method of calculation does not seem feasible in this case. Thus no systematic application of many-body perturbation theory has yet been attempted. However, the propagator formalism of Luttinger and Ward[2] is well suited to this problem. By using such a formalism one performs a partial summation of the perturbation series. Also the low-temperature expansion of the free energy can be obtained conveniently. In addition, long wavelength divergences can be explicitly avoided. Finally, the use of diagrammatic techniques allows one to examine terms of arbitrarily high order in the perturbation. Our treatment is incomplete in that we assume that the kinematic interaction can be neglected and that the perturbation series is a useful one.

We treat the case of an isotropic body-centered cubic Heisenberg antiferromagnet whose Hamiltonian is

$$\mathcal{H}=2J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j \quad (1)$$

in the usual notation. Using Oguchi's transformation[3] one can express this in terms of the boson operators $a_\mathbf{k}$ and $b_\mathbf{k}$ as $\mathcal{H}=E^0+\mathcal{H}_0+V$, where $E^0=-NzJS^2$ and,

$$\mathcal{H}_0=16JS\sum a_\mathbf{k}^+a_\mathbf{k}+b_\mathbf{k}^+b_\mathbf{k}+\gamma_\mathbf{k}a_\mathbf{k}^+b_{-\mathbf{k}}^++\gamma_\mathbf{k}a_\mathbf{k}b_{-\mathbf{k}}, \quad (2)$$

$$V=-16JN^{-1}\sum[2\gamma_{\mathbf{k}-\mathbf{k}'}a_\mathbf{k}^+a_{\mathbf{k}'}b_{\mathbf{k}''}^+b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}''}$$
$$+\gamma_{\mathbf{k}'}a_\mathbf{k}^+b_{\mathbf{k}'}a_{\mathbf{k}''}a_{\mathbf{k}-\mathbf{k}'-\mathbf{k}''}+\gamma_\mathbf{k}a_\mathbf{k}^+b_{\mathbf{k}'}^+b_{\mathbf{k}''}^+b_{\mathbf{k}+\mathbf{k}'+\mathbf{k}''}], \quad (3)$$

where $\gamma_\mathbf{k}=\cos(k_xa/2)\cos(k_ya/2)\cos(k_za/2)$. To diagonalize $\mathcal{H}_0$ one introduces boson operators $c_\mathbf{k}$ and $d_\mathbf{k}$ which are given as

$$c_\mathbf{k}=p_\mathbf{k}a_\mathbf{k}-q_\mathbf{k}b_{-\mathbf{k}}^+, \qquad d_{-\mathbf{k}}=-q_\mathbf{k}a_\mathbf{k}^++p_\mathbf{k}b_{-\mathbf{k}}, \quad (4)$$

$$p_\mathbf{k}^2=[(1-\gamma_\mathbf{k}^2)^{-\frac{1}{2}}+1]/2, \qquad q_\mathbf{k}^2=[(1-\gamma_\mathbf{k}^2)^{-\frac{1}{2}}-1]/2. \quad (5)$$

In this cd representation $\mathcal{H}_0$ takes the simple form

$$\mathcal{H}_0=\sum e_\mathbf{k}(c_\mathbf{k}^+c_\mathbf{k}+d_\mathbf{k}^+d_\mathbf{k}), \qquad e_\mathbf{k}\equiv e(\mathbf{k})=16JS(1-\gamma_k^2)^{\frac{1}{2}}. \quad (6)$$

Normally the next step would be to express V in the cd representation and apply perturbation theory. However, the perturbation then takes on an extremely unwieldy form involving terms which become infinite for $k=0$, since $p_\mathbf{k}$ and $q_\mathbf{k}$ vary as $k^{-\frac{1}{2}}$ for small k. Instead we leave the perturbation in the ab representation and apply the propagator formalism of Luttinger and Ward.[2]

For this purpose we consider the following relations:

$$\langle P[a_\mathbf{k}^+(\beta_1)a_{\mathbf{k}'}(\beta_2)]\rangle =-\beta^{-1}\delta_{\mathbf{k}\mathbf{k}'}\sum_m S^0(\mathbf{k},z_m)_{aa}\exp\{z_m(\beta_1-\beta_2)\}, \quad (7a)$$

$$\langle P[a_\mathbf{k}^+(\beta_1)b_{-\mathbf{k}'}^+(\beta_2)]\rangle =-\beta^{-1}\delta_{\mathbf{k}\mathbf{k}'}\sum_m S^0(\mathbf{k},z_m)_{ab}\exp\{z_m(\beta_1-\beta_2)\}, \quad (7b)$$

$$\langle P[a_\mathbf{k}(\beta_2)b_{-\mathbf{k}'}(\beta_1)]\rangle =-\beta^{-1}\delta_{\mathbf{k}\mathbf{k}'}\sum_m S^0(\mathbf{k},z_m)_{ba}\exp\{z_m(\beta_1-\beta_2)\}, \quad (7c)$$

$$\langle P[b_\mathbf{k}^+(\beta_2)b_{-\mathbf{k}'}(\beta_1)]\rangle =-\beta^{-1}\delta_{\mathbf{k}\mathbf{k}'}\sum_m S^0(\mathbf{k},z_m)_{bb}\exp\{z_m(\beta_1-\beta_2)\}, \quad (7d)$$

where P is the time-ordering operator, the boson operators are the usual time-dependent operators, the bracket indicates an average over a canonical distribution at temperature $kT=\beta^{-1}$, $z_m\equiv z(m)=2m\pi i/\beta$, and m is summed from $-\infty$ to $+\infty$. The matrix $\mathbf{S}^0(\mathbf{k},z)$ is called the unperturbed propagator and its

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[1] F. J. Dyson, Phys. Rev. **102,** 1217 (1956).
[2] J. M. Luttinger and J. C. Ward, Phys. Rev. **118,** 1417 (1960); J. M. Luttinger, Phys. Rev. **119,** 1153 (1960); **121,** 942 (1961).
[3] T. Oguchi, Progr. Theoret. Phys. (Kyoto) **22,** 721 (1961).

components are

$$S_{aa}=(z+16JS)/(z^2-e_k^2)$$
$$S_{ab}=(-16JS\gamma_k)/(z^2-e_k^2), \quad (8a)$$
$$S_{ba}=(-16JS\gamma_k)/(z^2-e_k^2)$$
$$S_{bb}=(-z+16JS)/(z^2-e_k^2). \quad (8b)$$

The free energy can be expressed diagrammatically in terms of this propagator as follows. The nth-order term for $\ln(Z/Z_0)$ is constructed from diagrams according to the following rules: Number n points. From each point draw two outgoing lines representing a_k^+ or b_{-k} operators and draw two ingoing lines representing a_k or b_{-k}^+ operators. Connect ingoing and outgoing lines together in pairs and label each line j with values of momentum $\mathbf{k}_j$ and "energy" $z(m_j)$, and give each line indices a_j and b_j at each vertex. At each vertex energy and momentum are conserved. For a line j with indices α and β take a factor $S^0[\mathbf{k}_j, z(m_j)]_{\alpha\beta}$ and for each vertex include the appropriate matrix element of the perturbation. Include also an over-all factor $(\beta^n n!)^{-1}$, sum over all propagator indices α_j and β_j, momenta $\mathbf{k}_j$, energies $z(m)_j$, and over-all connected diagrams.

One defines the true propagator $S(\mathbf{k}, z)_{\alpha\beta}$ as what one gets by applying the above rules to connected diagrams when one line of momentum $\mathbf{k}$ and energy z is cut in half and the free ends assigned indices α and β. One also defines the proper self-energy $G(\mathbf{k}, z)_{\alpha\beta}$ as the contribution from proper diagrams when the line with indices α and β is removed; then

$$\mathbf{S}(\mathbf{k}, z)=[S^0(\mathbf{k}, z)^{-1}-\mathbf{G}(\mathbf{k}, z)]^{-1}. \quad (9)$$

One can show that the free energy is stationary with respect to variations in the proper self-energy and that the lowest-order temperature dependence of the free energy is given by

$$F^{(1)}=\beta^{-1}\sum_k\sum_m Tr\ln[-\mathbf{S}^0(\mathbf{k}, z_m)^{-1}+\mathbf{G}(\mathbf{k}, z_m)], \quad (10)$$

where $\mathbf{G}(\mathbf{k}, z_m)$ is evaluated at $T=0$. By a suitable contour integration one can derive the formula

$$F^{(1)}=-2\beta^{-1}\sum_{\mathbf{k}}\ln[1-\exp(-\beta\,|\,E_k\,|\,)], \quad (11)$$

where E_k is the true single-particle energy which satisfies

$$\mathrm{Det}\,|\,\mathbf{S}^0(\mathbf{k}, E_k)^{-1}-\mathrm{Re}G(k, E_k)\,|=0.$$

In order to discuss the properties of the proper self-energy it is convenient to express it in terms of time ordered diagrams in which the vertices are assigned "times" t_v and these times are permuted to give $n!$ time-ordered diagrams for each original diagram. The contribution to $\mathbf{G}(\mathbf{k}, z)$ is made up of the following factors: an over-all factor $n!^{-1}$, the appropriate matrix element for each vertex, a factor

$$[z_j^2-e(\mathbf{k}_j)^2]\mathbf{S}^0(\mathbf{k}_j, z_j)/2e(\mathbf{k}_j)$$

evaluated at $z_j=e(\mathbf{k}_j)$ for lines j going towards later times and at $z_j=-e(\mathbf{k}_j)$ for lines going towards earlier times, and a factor D_v^{-1} for each time interval, where D_v is the sum of the energies of all lines present in the time interval between t_v and t_{v+1}. From the appearance of the factor $e(\mathbf{k}_j)^{-1}$ one might conclude that the long wavelength divergence is still present; however, by a suitable pairing of diagrams one can show that the sum of the integrands of the two paired diagrams is regular for any $k_j=0$.

Furthermore, by examining the diagrammatic series for the proper self-energy, one can easily see that the excitation energy can not involve even powers of k, and that the two spin wave branches are degenerate. Aside from higher-order nonanalytic terms of the form $k^n\log k$ whose analysis is rather difficult and is not yet complete, the excitation spectrum is of the form

$$E_k=A(ak)+B(\theta_k, \phi_k)(ak)^2+C(\theta_k, \phi_k)(ak)^5. \quad (13)$$

One finds using Eq. (11) that the free energy is of the form

$$F=A'T^4+B'T^6+C'T^8. \quad (14)$$

The quantities A, B, and C can be calculated diagrammatically. From Eqs. (2) and (3) one sees that these quantities will be given by a power series in $1/S$, of which Oguchi[4] has calculated the terms up to order $1/S$. These results can be obtained by considering diagrams with a single vertex. From the diagrams with two vertices we find

$$A=8JS(1+c/2S)(1-0.005/S^2). \quad (15)$$

Thus it seems that perturbation theory converges rapidly for a three-dimensional lattice.

For a ferromagnet this stage of the approximation gives no correction to the noninteracting spin waves, since for $T=0$ the proper self-energy vanishes. To obtain the approximation which gives Dyson's T^5 term one would have to give a more complete formula for the free energy and also calculate the proper self-energy at nonzero temperature.

The advantages of the present formulation are several. It enables one to eliminate the long wavelength divergence in a simple way. It also allows one to choose an unperturbed Hamiltonian which is closer to the true Hamiltonian than in some other calculations. This method is amenable to summation procedures and can also provide a consistent treatment of the kinematic effect as we will show elsewhere. Accordingly, although the numerical results may not be impressive, we feel that this formulation opens the way to more systematic and comprehensive treatments of this problem.

[4] T. Oguchi, Phys. Rev. **117**, 117 (1960).