Anisotropic Heisenberg Linear Chain at Nonzero Temperature*

J. T. HUNT AND M. D. GIRARDEAU
Institute of Theoretical Science and Department of Physics, University of Oregon, Eugene, Oregon

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The statistical mechanics of the anisotropic Heisenberg chain is treated by the Bogolyubov variational method, taking the anisotropic X-Y model as trial Hamiltonian. The free energy of the antiferromagnet is well behaved for all values of the temperature and anisotropy, reducing in the isotropic case to results obtained previously by Katsura and Bulaevskii. The behavior of the ferromagnet in the isotropic case is similar to that found by Katsura.

1. INTRODUCTION

IN spite of the voluminous literature on the Heisenberg model of ferromagnetism, there are still few accurate results known at nonzero temperature. In the present paper we study the anisotropic Heisenberg linear chain at nonzero temperature, both for the ferromagnetic and antiferromagnetic cases. Our method of calculation consists of an application of the Bogolyubov variational principle for the free energy. This variational principle yields a rigorous upper bound to the free energy at all temperatures and for all values of the exchange and anisotropy parameters; by minimizing this upper bound with respect to variational parameters, one obtains the best approximation to the free energy consistent with the variational ansatz.

The formulation of the variational principle and analytical evaluation of the bound are carried out in Sec. 2, and the variational equations arising through minimization of the bound are derived. In Secs. 3–6 the Ising limit, ground-state energy, and low- and high-temperature behavior are evaluated and compared with the known results. In the remainder of the paper, the results of numerical calculations of the optimal bound are presented for all temperatures and values of the exchange and anisotropy parameters.

2. FORMULATION

We write the Hamiltonian of the anisotropic Heisenberg linear chain in the form

$$H=-2J\sum_{j=1}^{N-1}[(1+\gamma)S_j^xS_{j+1}^x+(1-\gamma)(S_j^yS_{j+1}^y+S_j^zS_{j+1}^z)],\quad(1)$$

where $\gamma, -1\leq\gamma\leq 1$, is the anisotropy parameter, J the nearest-neighbor exchange constant, and $\mathbf{S}_j$ the spin operator on site j; the total spin on each site is $\frac{1}{2}$. The Helmholtz free energy F is defined by

$$e^{-\beta F}=\mathrm{Tr}e^{-\beta H}.\quad(2)$$

If H_0 is any "trial Hamiltonian" of the system, i.e., any Hermitian function of the $\mathbf{S}_j$, then the Bogolyubov variational principle[1] states that the true free energy is always less than a "trial free energy" F_{trial}:

$$F\leq F_{\mathrm{trial}}\equiv F_0+\langle H-H_0\rangle_0.\quad(3)$$

Here F_0 is the free energy of H_0,

$$\exp(-\beta F_0)=\mathrm{Tr}\exp(-\beta H_0),\quad(4)$$

and the angular bracket denotes an average in the canonical ensemble of H_0:

$$\langle H-H_0\rangle_0\equiv\frac{\mathrm{Tr}[(H-H_0)\exp(-\beta H_0)]}{\mathrm{Tr}\exp(-\beta H_0)}.\quad(5)$$

As in the case of the quantum-mechanical variational principle for the ground-state energy, of which (3) is a generalization to nonzero temperature, one lets H_0 depend on variational parameters and minimizes F_{trial} with respect to these parameters so as to obtain an optimal upper bound.

We shall choose H_0 to be the Hamiltonian of the anisotropic XY model, which is exactly soluble[2,3]:

$$H_0=-2J'\sum_{j=1}^{N-1}[(1+\tilde{\gamma})S_j^xS_{j+1}^x+(1-\tilde{\gamma})S_j^yS_{j+1}^y].\quad(6)$$

Our somewhat unconventional choice of the x axis as the "longitudinal" direction and hence the y and z axes as "transverse" in (1) is made in order to facilitate comparison with the work of Lieb, Schultz, and Mattis, who chose the x axis as longitudinal in (6). The variational parameters are J' and $\tilde{\gamma}$; there is no reason to expect the best choice of these parameters to be the same as γ and J except in certain limiting cases.

By (1) and (6) one has

$$\langle H-H_0\rangle_0=-2\sum_{j=1}^{N-1}\{[J(1+\gamma)-J'(1+\tilde{\gamma})]\langle S_j^xS_{j+1}^x\rangle_0+[J(1-\gamma)-J'(1-\tilde{\gamma})]\langle S_j^yS_{j+1}^y\rangle_0+J(1-\gamma)\langle S_j^zS_{j+1}^z\rangle_0\}.\quad(7)$$

Now by (4) and (5)

$$\partial F_0/\partial p=\langle\partial H_0/\partial p\rangle_0,\quad(8)$$

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[1] N. N. Bogolyubov, unpublished work cited in footnote 4 of V. V. Tolmachev, Dokl. Acad. Nauk. SSSR **134**, 1324 (1960) [English transl.: Soviet Phys.—Doklady **5**, 984 (1961)].

[2] E. Leib, T. Shultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 409 (1961).

[3] S. Katsura, Phys. Rev. **127**, 1508 (1962).

where p is any c-number parameter in H_0. A little straightforward algebra then yields

$$\langle H-H_0\rangle_0=(J-J')\frac{\partial F_0}{\partial J'}+\frac{J}{J'}(\gamma-\tilde{\gamma})\frac{\partial F_0}{\partial\tilde{\gamma}}-2J(1-\gamma)\sum_{j=1}^{N-1}\langle S_j^zS_{j+1}^z\rangle_0. \quad (9)$$

Thus the only nontrivial term in F_{trial} is that involving

$$\langle S_j^zS_{j+1}^z\rangle_0.$$

Our H_0 is related to the Hamiltonian H_γ of Lieb, Schultz, and Mattis[4] by

$$H_0=-2J'H_{\tilde{\gamma}}. \quad (10)$$

These authors first introduce raising and lowering operators a_j, $a_j^\dagger$ by the usual transformation

$$a_j^\dagger=S_j^x+iS_j^y, \qquad a_j=S_j^x-iS_j^y,$$
$$S_j^x=\tfrac{1}{2}(a_j+a_j^\dagger), \qquad S_j^y=\tfrac{1}{2}i(a_j-a_j^\dagger),$$
$$S_j^z=a_j^\dagger a_j-\tfrac{1}{2}. \quad (11)$$

These obey Pauli commutation and anticommutation rules:

$$[a_j,a_j^\dagger]_+=1, \qquad (a_j)^2=(a_j^\dagger)^2=0,$$
$$[a_j,a_l^\dagger]_-=[a_j^\dagger,a_l^\dagger]_-=[a_j,a_l]_-=0, \qquad j\neq l. \quad (12)$$

Fermion annihilation and creation operators c_j, $c_j^\dagger$ are then introduced by the Jordan–Wigner transformation

$$c_j=\exp\Big[i\pi\sum_{l=1}^{j-1}a_l^\dagger a_l\Big]a_j,$$
$$c_j^\dagger=a_j^\dagger\exp\Big[-i\pi\sum_{l=1}^{j-1}a_l^\dagger a_l\Big],$$
$$a_j=\exp\Big[-i\pi\sum_{l=1}^{j-1}c_l^\dagger c_l\Big]c_j,$$
$$a_j^\dagger=c_j^\dagger\exp\Big[i\pi\sum_{l=1}^{j-1}c_l^\dagger c_l\Big]. \quad (13)$$

Then c_j, $c_j^\dagger$ satisfy the usual Fermi anticommutation rules:

$$[c_j,c_l^\dagger]_+=\delta_{jl},$$
$$[c_j,c_l]_+=[c_j^\dagger,c_l^\dagger]_+=0. \quad (14)$$

Furthermore,

$$a_j^\dagger a_j=c_j^\dagger c_j, \qquad 1\leq j\leq N$$
$$a_j^\dagger a_{j+1}=c_j^\dagger c_{j+1}, \qquad i\leq j\leq N-1$$
$$a_j^\dagger a_{j+1}^\dagger=c_j^\dagger c_{j+1}^\dagger, \qquad 1\leq j\leq N-1. \quad (15)$$

[4] E. Leib, T. Shultz, and D. Mattis, Ref. 2, p. 409.

Thus

$$H_0=-J'\sum_{j=1}^{N-1}[(c_j^\dagger c_{j+1}+\tilde{\gamma}c_j^\dagger c_{j+1}^\dagger)+\text{H.c.}]. \quad (16)$$

Furthermore

$$S_j^zS_{j+1}^z=(c_j^\dagger c_j-\tfrac{1}{2})(c_{j+1}^\dagger c_{j+1}-\tfrac{1}{2}). \quad (17)$$

In order to simplify the analysis, it is desirable to replace (6) by the cyclic Hamiltonian

$$H_0=-J'\sum_{j=1}^{N}[(c_j^\dagger c_{j+1}+\tilde{\gamma}c_j^\dagger c_{j+1})+\text{H.c.}], \quad (18)$$

where

$$c_{N+1}\equiv c_1, \qquad c_{N+1}^\dagger\equiv c_1^\dagger. \quad (19)$$

Similarly, we replace

$$\sum_1^{N-1}S_j^zS_{j+1}^z \quad\text{by}\quad \sum_1^{N}S_j^zS_{j+1}^z. \quad (20)$$

As pointed out by Lieb, Shultz, and Mattis, such a change of boundary conditions is allowable, since the resultant change in the free energy is only $O(1)$, hence is negligible in the thermodynamic limit [where $F=O(N)$]. Then (3) and (9) become

$$F\leq F_{\text{trial}}=F_0+(J-J')\frac{\partial F_0}{\partial J}+\frac{J}{J'}(\gamma-\tilde{\gamma})\frac{\partial F_0}{\partial\tilde{\gamma}}-2J(1-\gamma)\sum_{j=1}^{N}\langle(c_j^\dagger c_j-\tfrac{1}{2})(c_{j+1}^\dagger c_{j+1}-\tfrac{1}{2})\rangle_0, \quad (21)$$

where F_0 and $\langle\ \rangle_0$ are evaluated in the ensemble of the cyclic Hamiltonian (18), (19).

The expression for F_0 can be read off from the work of Lieb, Schultz, and Mattis[2] and of Katsura[3]; it is

$$F_0(J',\tilde{\gamma},\beta)=-NKT\Big[\ln 2+\frac{2}{\pi}\int_0^{\pi/2}dk\ln\cosh(J'\beta\Lambda_k)\Big], \quad (22)$$

with

$$\Lambda_k=(\cos^2k+\tilde{\gamma}^2\sin^2k)^{1/2}. \quad (23)$$

However, in order to evaluate the explicit $\langle\ \rangle_0$ in (21) it is necessary to know the expression for the bracketed operator in the representation in which H_0 is diagonal. Since the representation we have found most convenient in evaluating (21) is slightly different from those of Refs. 2 and 3, we shall repeat the diagonalization of H_0 here, following a Bogolyubov–Valatin transformation method analogous to that of Katsura.

First we transfer to running-wave annihilation and creation operators α_k, $\alpha_k^\dagger$ by the unitary transformation

$$c_j=N^{-1/2}\sum_k\alpha_ke^{ikj}, \qquad c_j^\dagger=N^{-1/2}\sum_k\alpha_k^\dagger e^{-ikj}, \quad (24)$$

where

$$k=2\pi m/N,$$
$$m=-\tfrac{1}{2}(N-1),-\tfrac{1}{2}(N-1)+1,\cdots,0,1,\cdots,\tfrac{1}{2}(N-1). \quad (25)$$

For simplicity, we assume N to be odd. Then, using the relation

$$\sum_{j=1}^{N} \exp[i(k'-k)j]=N\delta_{k',k}, \tag{26}$$

it is easy to show that (18) becomes

$$H_0=-J'\sum_k [2\alpha_k{}^\dagger\alpha_k \cos k+\tilde{\gamma}(\alpha_k{}^\dagger\alpha_{-k}{}^\dagger e^{ik}+\alpha_{-k}\alpha_k e^{-ik})]. \tag{27}$$

Similarly, one can transform the quartic operator occurring in (21):

$$\sum_{j=1}^{N} (c_j{}^\dagger c_j-\tfrac{1}{2})(c_{j+1}{}^\dagger c_{j+1}-\tfrac{1}{2})$$

$$=\tfrac{1}{4}N-\sum_{j=1}^{N} c_j{}^\dagger c_j-\sum_{j=1}^{N} c_j{}^\dagger c_{j+1}{}^\dagger c_{j+1}c_j$$

$$=\tfrac{1}{4}N-\sum_k \alpha_k{}^\dagger\alpha_k+N^{-1}\sum_{qkk'} e^{iq}\alpha_{k+q}{}^\dagger\alpha_{k'-q}{}^\dagger\alpha_{k'}\alpha_k. \tag{28}$$

In order to put H_0 into a form in which it can be diagonalized by a Bogolyubov–Valatin transformation, we note that since the sum in (27) is over both positive and negative values of k, the off-diagonal terms for k and $-k$ can be combined into an even function of k:

$$\alpha_k{}^\dagger\alpha_{-k}{}^\dagger e^{ik}+\alpha_{-k}{}^\dagger\alpha_k{}^\dagger e^{-ik}=\alpha_k{}^\dagger\alpha_{-k}{}^\dagger(e^{ik}-e^{-ik})$$
$$=2i\alpha_k{}^\dagger\alpha_{-k}{}^\dagger \sin k. \tag{29}$$

Thus (27) becomes

$$H_0=-J'\sum_k [2\alpha_k{}^\dagger\alpha_k \cos k+i\tilde{\gamma}(\alpha_k{}^\dagger\alpha_{-k}{}^\dagger-\alpha_{-k}\alpha_k)\sin k]. \tag{30}$$

To diagonalize (30), we make a Bogolyubov-Valatin unitary transformation to new Fermi operators β_k, $\beta_k{}^\dagger$. This transformation can be written in the form

$$\alpha_k=\frac{\beta_k+\varphi_k\beta_{-k}{}^\dagger}{(1+|\varphi_k|^2)^{1/2}},\qquad \alpha_k{}^\dagger=\frac{\beta_k{}^\dagger+\varphi_k{}^*\beta_{-k}}{(1+|\varphi_k|^2)^{1/2}}, \tag{31}$$

where φ_k is a complex c-number function which is odd:

$$\varphi_{-k}=-\varphi_k. \tag{32}$$

One finds that the off-diagonal terms in H_0 in the new representation (those proportional to $\beta_k{}^\dagger\beta_{-k}{}^\dagger$ and $\beta_{-k}\beta_k$) vanish provided that

$$\varphi_k=(\pm\Lambda_k-\cos k)/i\tilde{\gamma}\sin k, \tag{33}$$

where Λ_k is given by (23). The choice of the plus or minus sign in (33) (the sign of the square root in the solution of the quadratic equation for φ_k) should be made so that φ_k vanishes as $\tilde{\gamma}\to 0$, since the off-diagonal terms in (30) vanish in that limit. Thus one should choose the sign of Λ_k to be the same as that of $\cos k$. Then H_0 takes the diagonal form[5]

$$H_0=-2J'\sum_k (\pm\Lambda_k\beta_k{}^\dagger\beta_k). \tag{34}$$

The free energy is then

$$F_0=-KT\ln \operatorname{Tr}\exp(-\beta H_0)$$
$$=-KT\ln\operatorname{Tr}\exp[2\beta J'\sum_k \pm\Lambda_k\beta_k{}^\dagger\beta_k]$$
$$=-KT\sum_k \ln[1+\exp(\pm 2\beta J'\Lambda_k)]$$
$$=-KT\sum_k \ln[2\exp(\pm\beta J'\Lambda_k)\cosh(\beta J'\Lambda_k)]$$
$$=-\sum_k [\beta^{-1}\ln 2\pm J'\Lambda_k+\beta^{-1}\ln\cosh(\beta J'\Lambda_k)]. \tag{35}$$

Changing the sum to an integral according to the prescription

$$\sum_1 \to \frac{N}{2\pi}\int_{-\pi}^{\pi} dk$$

valid in the limit $N\to\infty$, noting that the integral of Λ_k vanishes,[5] and using the symmetry of Λ_k, one obtains precisely the result (22) of Lieb, Schultz, and Mattis. Taking the limit $\beta\to\infty$ in (22), one obtains the ground-state energy

$$E_0(J',\tilde{\gamma})=-2N\pi^{-1}|J'|\int_0^{1/2\pi} dk\Lambda_k$$
$$=-2N\pi^{-1}|J'|E(1-\tilde{\gamma}^2);\qquad \tilde{\gamma}\le 1$$
$$=-2N\pi^{-1}|J'||\tilde{\gamma}|E\left(\frac{\tilde{\gamma}^2-1}{\tilde{\gamma}^2}\right);\qquad |\tilde{\gamma}|\ge 1, \tag{36}$$

where E is the complete elliptic integral of the second kind. This agrees with Eq. (2.21) of Lieb, Schultz, and Mattis.

The thermal average of the transverse term [the explicit $\langle\ \rangle_0$ in (21)], can be evaluated with the aid of Matsubara's theorem,[6,7] according to which the thermal average of any product of annihilation and creation operators in an ensemble appropriate to independent fermions and/or bosons can be expressed in terms of products of *contractions*, each contraction being the thermal average of a product of only two operators, each linear in annihilation and creation operators. Since the transformation (31) conserves momentum, the only such contractions which are nonzero are those which conserve momentum. One thus finds

$$\sum_{j=1}^{N} \langle(c_j{}^\dagger c_j-\tfrac{1}{2})(c_{j+1}{}^\dagger c_{j+1}-\tfrac{1}{2})\rangle_0$$
$$=\tfrac{1}{4}N-\sum_k \langle\alpha_k{}^\dagger\alpha_k\rangle_0+N^{-1}\sum_{q,k} e^{iq}\langle\alpha_{k+q}{}^\dagger\alpha_{-k-q}{}^\dagger\rangle_0\langle\alpha_{-k}\alpha_k\rangle_0$$
$$+N^{-1}\sum_{k,k1}\{1-\exp[i(k-k')]\}\langle\alpha_k{}^\dagger\alpha_k\rangle_0\langle\alpha_{k1}{}^\dagger\alpha_{k1}\rangle_0. \tag{37}$$

To evaluate the various contractions occurring in (37)

[5] The constant term in H_0 vanishes since $\Sigma_k \cos k$ vanishes by symmetry (k runs from $-\pi$ to π), and by aforementioned choice of signs in (33) the sum $\Sigma_k\pm\Lambda_k$ also vanishes.

[6] T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955).

[7] C. Bloch and C. deDominicis, Nucl. Phys. **7**, 459 (1958), Sec. 3.

we note that, after the α_k, $\alpha_k^\dagger$ are expressed in terms of β_k, $\beta_k^\dagger$, only the diagonal contractions $\langle\beta_k^\dagger\beta_k\rangle_0$ and $\langle\beta_k\beta_k^\dagger\rangle_0$ are nonvanishing. Thus, using (31), one finds

$$\langle\alpha_k^\dagger\alpha_k\rangle_0=(1+|\varphi_k|^2)^{-1}[\langle\beta_k^\dagger\beta_k\rangle_0+|\varphi_k|^2\langle\beta_{-k}\beta_{-k}^\dagger\rangle_0],$$
$$\langle\alpha_k^\dagger\alpha_{-k}^\dagger\rangle_0=(1+|\varphi_k|^2)^{-1}\varphi_k^*[\langle\beta_{-k}\beta_{-k}^\dagger\rangle_0-\langle\beta_k^\dagger\beta_k\rangle_0],$$
$$\langle\alpha_{-k}\alpha_k\rangle_0=(1+|\varphi_k|^2)^{-1}\varphi_k[\langle\beta_{-k}\beta_{-k}^\dagger\rangle_0-\langle\beta_k^\dagger\beta_k\rangle_0]. \quad (38)$$

By (34) and standard arguments one has

$$\langle\beta_k^\dagger\beta_k\rangle_0=[\exp(\mp 2\beta J'\Lambda_k)+1]^{-1},$$
$$\langle\beta_k\beta_k^\dagger\rangle_0=1-\langle\beta_k^\dagger\beta_k\rangle_0=[\exp(\pm 2\beta J\Lambda_k)+1]^{-1}. \quad (39)$$

Thus by (33),

$$\langle\alpha_k^\dagger\alpha_k\rangle_0=\tfrac{1}{2}[1+\Lambda_k^{-1}\cos k\tanh(\beta J'\Lambda_k)],$$
$$\langle\alpha_k^\dagger\alpha_{-k}^\dagger\rangle_0=-\tfrac{1}{2}i\tilde{\gamma}\Lambda_k^{-1}\sin k\tanh(\beta J'\Lambda_k),$$
$$\langle\alpha_{-k}\alpha_k\rangle_0=\tfrac{1}{2}i\tilde{\gamma}\Lambda_k^{-1}\sin k\tanh(\beta J'\Lambda_k). \quad (40)$$

Substituting these expressions into (37) and thence into (21), one finds,[8] after converting k sums to integrals,

$$F_{\text{trial}}/JN=2\pi^{-1}\Bigg\{-2T\int_0^{\pi/2}dk\,\ln\left[2\cosh\left(\frac{p}{2T^*}\Lambda_k\right)\right]$$
$$-(\gamma-\tilde{\gamma})\tilde{\gamma}\int_0^{\pi/2}dk\,\Lambda_k\sin^2 k\tanh\left(\frac{p}{2T^*}\Lambda_k\right)$$
$$-(1-p)\int_0^{\pi/2}dk\,\Lambda_k^{-1}\tanh\left(\frac{p}{2T^*}\Lambda_k\right)$$
$$-(1-\gamma)\pi N^{-1}Z(p,\tilde{\gamma},T^*)\Bigg\}, \quad (41)$$

where $p=J'/J$, $1/T^*=2\beta J$, and

$$Z(p,\tilde{\gamma},T)=N[\tilde{\gamma}^2S^2(p,\tilde{\gamma},T^*)-C^2(p,\tilde{\gamma},T^*)], \quad (42)$$

$$S=\pi^{-1}\int_0^{\pi/2}dk\,\Lambda_k^{-1}\sin^2 k\tanh\left(\frac{p}{2T^*}\Lambda_k\right), \quad (43)$$

$$C=\pi^{-1}\int_0^{\pi/2}\Lambda_k^{-1}\cos^2 k\tanh\left(\frac{p}{2T^*}\Lambda_k\right). \quad (44)$$

T^* negative corresponds to the antiferromagnet and T^* positive to the ferromagnet. The minimum of the trial free energy is obtained by solving $\partial F_{\text{trial}}/\partial\tilde{\gamma}=0$ and $\partial F_{\text{trial}}/\partial p=0$ for $\tilde{\gamma}$ and p, the solution of these two equations giving the extrema of the free energy. The derivatives of F_{trial} with respect to $\tilde{\gamma}$ and p vanish if the following two equations are satisfied:

$$\gamma-\tilde{\gamma}+2\pi^{-1}(1-\gamma)\tilde{\gamma}\int_0^{\pi/2}dk\,\Lambda_k^{-1}\tanh\left(\frac{p}{2T^*}\Lambda_k\right)=0 \quad (45)$$

$$-(1-p)+2\pi^{-1}(1-\gamma)\times\int_0^{\pi/2}dk\,\Lambda_k^{-1}\cos^2 k\tanh\left(\frac{p}{2T^*}\Lambda_k\right)=0. \quad (46)$$

Henceforth (45) and (46) will be referred to as the variational equations.

Using the relations (45) and (46), the expression for the trial free energy is found to be

$$F_{\text{trial}}/JN=F_0/JN-\tfrac{1}{2}(1-\gamma)^{-1}[(1-p)^2-(\tilde{\gamma}p-\gamma)^2] \qquad \tilde{\gamma}\pm 1, \quad (47)$$

where

$$(JN)^{-1}F_0=-4\pi^{-1}T^*\int_0^{\pi/2}dk\,\ln\left[2\cosh\left(\frac{p}{2T^*}\Lambda_k\right)\right].$$

To obtain an expression for the internal energy, we take as a definition

$$\text{internal energy}=d(\beta F_{\text{trial}})/d\beta, \quad (48)$$

$$\frac{d(\beta F_{\text{trial}})}{d\beta}=\frac{\partial}{\partial\beta}(\beta F_{\text{trial}})+\beta\left[\frac{\partial F_{\text{trial}}}{\partial p}\frac{dp}{d\beta}+\frac{\partial F_{\text{trial}}}{\partial\tilde{\gamma}}\frac{d\tilde{\gamma}}{d\beta}\right]. \quad (49)$$

But we have chosen $\partial F_{\text{trial}}/\partial p=\partial F_{\text{trial}}/\partial\tilde{\gamma}=0$ as the minimization conditions for F_{trial}. Therefore

$$d(\beta F_{\text{trial}})/d\beta=(\partial/\partial\beta)(\beta F_{\text{trial}}) \quad (50)$$
$$=\langle H\rangle_0+\beta(\partial/\partial\beta)\langle H-H_0\rangle_0. \quad (51)$$

But $(\partial/\partial\beta)\langle H-H_0\rangle_0=0$, since $\langle H-H_0\rangle_0$ does not contain β explicitly. Therefore

$$d(\beta F_{\text{trial}})/d\beta=\langle H\rangle_0=\text{internal energy}. \quad (52)$$

In terms of the variational parameters one obtains for the internal energy,

$$\langle H\rangle/JN=-\tfrac{1}{2}(1-\gamma)^{-1}[1-\gamma^2-(1-\tilde{\gamma}^2)p^2], \qquad \gamma\pm 1. \quad (53)$$

3. ISING LIMIT

In the Ising limit, $\gamma=1$, the variational parameters are $\tilde{\gamma}=1$ and $p=1$. In this limit the trial Hamiltonian, H_0, and the actual Hamiltonian of the system are identical. Therefore we obtain the exact values for all thermodynamic quantities of interest.

$$(1/JN)\langle H\rangle_0^{\text{Ising}}=-\tanh(1/2T^*); \quad (54)$$

$$(1/JN)F^{\text{Ising}}=-2T^*\ln 2\cosh(p/2T^*). \quad (55)$$

Defining $c=(1/JN)(\partial\langle H\rangle_0/\partial T^*)$, which is the specific heat measured in units of $(2/Nk)$, we obtain

$$c=\tfrac{1}{2}(T^*)^{-2}\,\text{sech}^2(1/2T^*). \quad (56)$$

[8] Use has been made of the fact

$$\int_{-\pi}^{\pi}dk\,\cos k\Lambda_k^{-1}\tanh(\beta J'\Lambda_k)=0,$$

due to the symmetry of $\cos k$ and Λ_k.

4. GROUND-STATE ENERGY

In the limit of zero temperature the free energy is equal to the ground-state energy:

$$\lim_{T\to 0} F_{\text{trial}} = \langle H \rangle_0,$$

$$E_{\text{trial}} = \langle H \rangle_0. \quad (57)$$

The values of p and $\tilde{\gamma}$ occurring in $\langle H\rangle_0$, which is given by Eq. (53), are the solution of zero-temperature variational equations

$$\gamma - \tilde{\gamma} + 2\pi^{-1}(1-\gamma)\tilde{\gamma}\,\text{sgn}(T^*) \int_0^{\pi/2} dk\, \Lambda_k^{-1} = 0, \quad (58)$$

$$-(1-p) + 2\pi^{-1}(1-\gamma)\,\text{sgn}(T^*) \int_0^{\pi/2} dk \cos^2 k\, \Lambda_k^{-1} = 0, \quad (59)$$

where we have used the relation

$$\lim_{T\to 0} \tanh[(p/2T^*)\,\Lambda_k] = \text{sgn}(T^*).$$

First we consider the ferromagnetic case where $\text{sgn}(T^*)=1$. For $0 \leq \gamma \leq 1$ the solution of (58) is $\tilde{\gamma}=1$. The trial ground-state energy is

$$E_{\text{trial}} = -\tfrac{1}{2}(1+\gamma); \qquad 0 \leq \gamma \leq 1. \quad (60)$$

This is the exact ground-state energy, corresponding to all spins aligned along the x axis. A simple proof that (60) is the exact ground-state energy is the following[9]:

Write the Hamiltonian as

$$H = -2J(1+\gamma)\left[\sum_j \{(1-\sigma)\, S_j^x S_{j+1}^x + \sigma \mathbf{S}_j \cdot \mathbf{S}_{j+1}\}\right], \quad (61)$$

where $\sigma = (1-\gamma)/(1+\gamma)$.

The totally aligned state gives the maximal eigenvalue of $S_j^x S_{j+1}^x$ and $\mathbf{S}_j\ \mathbf{S}_{j+1}$, yielding the minimum energy of the system. In the isotropic limit, $\gamma=0$, Eq. (58) has three solutions, $\tilde{\gamma}=\pm 1$ and $\tilde{\gamma}=0$. $\tilde{\gamma}=1$ corresponds to all spins aligned along the x axis and $\tilde{\gamma}=-1$ corresponding to all spins aligned along the y axis. These two solutions give the exact ground-state energy. The third solution, $\tilde{\gamma}=0$, gives a higher ground-state energy and is discarded. We now consider the region of anisotropy, $-1 \leq \gamma \leq 0$. Although $\tilde{\gamma}=1$ is a solution of (58) for all ferromagnetic anisotropy, it does not minimize the energy for $-1 \leq \gamma < 0$. The minimum energy was obtained by solving (58) numerically. The resulting energy is compared with the exact energy given by des Cloizeaux[10] in Fig. 1.

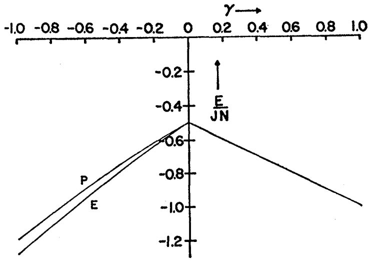

FIG. 1. Comparison of the variational ferromagnetic ground-state energy to the exact ground-state energy. E is the exact energy and P the present work.

The solution of (58) within this region of anisotropy yields $\tilde{\gamma} < -1$. Writing the trial Hamiltonian in the form

$$H_0 = -\sum_j (J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y), \quad (62)$$

where $J_x = -2J(1+\tilde{\gamma})$; $J_y = -2J(1-\tilde{\gamma})$, shows that the exchange constants J_x and J_y have opposite signs. In the classical sense, where the different components of spin commute, this means that the y component of the spins is interacting ferromagnetically, whereas the x component is antiferromagnetic. This description is similar to that given by des Cloizeaux.[10]

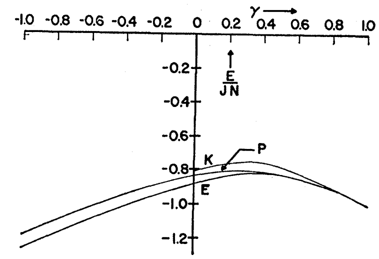

FIG. 2. Antiferromagnetic ground-state energy, E/JN, curves as a function of anisotropy, γ. E is the exact energy, K is Kasteleijn's variational energy, and P is present work.

For the antiferromagnet, $\text{sgn}(T^*)=-1$. Equation (58) was solved numerically and Fig. (2) shows that the resulting energy is closer to the exact energy[10,11] than the variational calculation of Kasteleijn.[12]

[*Note added in proof.* The vertical axis of Fig. 2 should be relabeled $E/|J|N$, the vertical axis of Fig. 3 should be relabeled $\Delta/2|J|$, and the vertical axis of Fig. 6 should be relabeled $\langle H\rangle/|J|N$.]

As can be seen from Figs. (1) and (2), there is good agreement between our ground-state energy and the exact result. The deviation in energy from the exact result is less than 8% for all values of exchange constant J, and anisotropy γ.

5. LOW-TEMPERATURE LIMIT

A perusal of the excitation spectrum of the XY model[13] shows that there is an energy gap between the ground state and the low-lying excited states of the system for $\tilde{\gamma}\neq 0$. Using this fact we can obtain a low-

[9] M. Wortis (private communication).

[10] J. des Cloizeaux and M. Gaudin, J. Math Phys. **7**, 1384 (1966).

[11] R. Orbach, Phys. Rev. **112**, 315 (1958).

[12] P. W. Kasteleijn, Physica **18**, 111 (1952).

[13] E. Leib, T. Shultz, and D. Mattis, Ref. 2, p. 414.

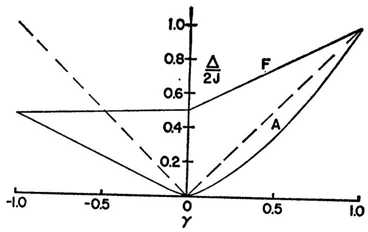

FIG. 3. Energy gap, $\Delta/2J$, between the ground state and first excited state as a function of anisotropy. "F" is the gap for the ferromagnet, "A" for the antiferromagnet, and the dashed curve is that of the anisotropic XY model.

temperature expansion for Z_0, the partition function, in the following manner.

$$Z_0 \equiv \sum_\alpha \langle \alpha \mid \exp(-\beta H_0) \mid \alpha \rangle \tag{63}$$

or since H_0 is diagonal we have $Z_0 = \sum_\alpha \exp(-\beta\epsilon_\alpha)$, where ϵ_α is the energy of state α. Hence

$$Z_0 = \exp(-\beta E_g) + \sum_\alpha{}' \exp(-\beta\epsilon_\alpha), \tag{64}$$

where E_g is the ground-state energy and the $\sum_\alpha{}'$ is a sum over the excited states of the system. Therefore, we can write $\epsilon_\alpha = E_g + \Delta + \epsilon_{\alpha'}$, where Δ is the difference in energy between the ground state and the first excited state of the system (the energy gap), and $\epsilon_{\alpha'}$ is the energy of the system measured relative to the energy of the first excited state.

Then the expression for Z_0 is

$$Z_0 = \exp(-\beta E_g) + \exp[-\beta(\Delta + E_g)] \sum_{\alpha'}{}' \exp(-\beta\epsilon_{\alpha'}), \tag{65}$$

$$Z_0 = \exp(-\beta E_g)[1 + \exp(-\beta\Delta) \sum_{\alpha'}{}' \exp(-\beta\epsilon_{\alpha'})]. \tag{66}$$

Hence

$$F_0 = -\beta^{-1} \ln Z_0, \tag{67}$$

$$F_0 = E_g + \beta^{-1} \ln[1 + \exp(-\beta\Delta) \sum_{\alpha'}{}' \exp(-\beta\epsilon_{\alpha'}], \tag{68}$$

which for large β becomes

$$F_0 \approx E_g + \beta^{-1} \exp(-\beta\Delta) \sum_{\alpha'}{}' \exp(-\beta\epsilon_{\alpha'}). \tag{69}$$

The expression for the energy gap, Δ, of the XY model is

$$\Delta = 2 \mid Jp\tilde{\gamma} \mid \quad \text{for} \quad \mid \tilde{\gamma} \mid \leq 1$$

and

$$\Delta = 2 \mid J \mid p \quad \text{for} \quad \mid \tilde{\gamma} \mid \geq 1.$$

Figure 3 is a plot of the zero-temperature variational energy gap of the anisotropic Heisenberg model.

Then using $\exp(-\beta\Delta)$ as a small expansion parameter, one can obtain expressions for F_{trial}, $\tilde{\gamma}$, p, internal energy, and the specific heat which are valid at low temperature.

An investigation of (58) and (59) as well as Fig. (3) shows that the energy gap at zero temperature vanishes only for the isotropic antiferromagnet. This special case is considered in Sec. 7. For a finite energy gap, the variational equations can be linearized in $\delta\tilde{\gamma}$ and δp with T^* treated as a parameter, $\delta\tilde{\gamma}$ and δp being the small change in $\tilde{\gamma}$ and p for $\mid T^* \mid \ll 1$.

First we consider the ferromagnet ($T^* > 0$) in the region of anisotropy $0 \leq \gamma \leq 1$. The quantities of interest, to first order in $\exp(-\beta\Delta)$ are

$$\delta\tilde{\gamma} = -4[(1-\gamma)/(1+\gamma)] \exp[-(1+\gamma)/2T^*], \tag{70}$$

$$\delta p = \tfrac{1}{2}[(1-\gamma)/(1+\gamma)](1+3\gamma) \exp[-(1+\gamma)/2T^*], \tag{71}$$

$$F_{\text{trial}}/JN = -\tfrac{1}{2}(1+\gamma) - 2T^* \exp[-(1+\gamma)/2T^*]. \tag{72}$$

For the antiferromagnet with $\gamma \neq 0$ and the ferromagnet with $-1 \leq \gamma < 0$, the values of the variational parameters at small temperature are obtained by linearizing Eqs. (45) and (46) and evaluating the resulting integrals by the method of steepest descents.

The results for the antiferromagnet are

$$\delta\tilde{\gamma} = \{a_1 \mid T^* \mid^{1/2} + a_2 \mid T^* \mid^{3/2} + O(\mid T^* \mid^{5/2})\} \times \exp(-p \mid \tilde{\gamma}/T^* \mid), \tag{73}$$

where

$$a_1 = \left\{\frac{(1-\gamma)\tilde{\gamma}^2}{(1-p)\tilde{\gamma}+\gamma}\right\} \{\mid \tfrac{1}{8}\pi p\tilde{\gamma}(1-\tilde{\gamma}^2) \mid\}^{-1/2};$$

$$a_2 = -\tfrac{1}{2} \mid p\tilde{\gamma} \mid^{-1} a_1, \tag{74}$$

$$\delta p = \{b_1 \mid T^* \mid^{1/2} + b_2 \mid T^* \mid^{3/2} + O(\mid T^* \mid^{5/2})\} \times \exp(-p \mid \tilde{\gamma}/T^* \mid), \tag{75}$$

where

$$b_1 = -\frac{1-\gamma}{(1-\tilde{\gamma}^2)} \left\{\frac{(1-2p)\tilde{\gamma}+\gamma}{(1-p)\tilde{\gamma}+\gamma}\right\} \{\mid \tfrac{1}{8}\tilde{\gamma}\pi p(1-\tilde{\gamma}^2) \mid\}^{-1/2},$$

$$b_2 = -\frac{1-\gamma}{p(1-\tilde{\gamma}^2)} \left[1 - \frac{1}{2 \mid \tilde{\gamma} \mid} \left\{\frac{\tilde{\gamma}(1-2p)+\gamma}{(1-p)\tilde{\gamma}+\gamma}\right\}\right] \times [\mid \tfrac{1}{8}\tilde{\gamma}\pi p(1-\tilde{\gamma}^2) \mid]^{1/2}, \tag{76}$$

$$F_{\text{trial}}/JN = E_{\text{trial}} - \{\mid \tfrac{1}{8}\pi p\tilde{\gamma}(1-\tilde{\gamma}^2) \mid\}^{-1/2} \mid T^* \mid^{3/2} \times \exp(-p \mid \tilde{\gamma}/T^* \mid). \tag{77}$$

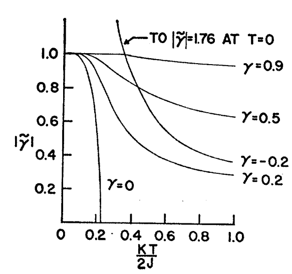

FIG. 4. The variational parameter $\tilde{\gamma}$ versus temperature for various anisotropy values in the ferromagnetic case.

For the ferromagnet we have

$$\delta\tilde{\gamma}=[c_1(T^*)^{1/2}+c_2(T^*)^{3/2}]\exp(-p/T^*), \quad (78)$$

where

$$c_1=\frac{(1-\gamma)\tilde{\gamma}^2\{\frac{1}{8}\pi p(\tilde{\gamma}^2-1)\}^{-1/2}}{\gamma+\tilde{\gamma}(1-p)}; \qquad c_2=-\tfrac{1}{2}p^{-1}c_1, \quad (79)$$

$$\delta p=[d_1(T^*)^{1/2}+d_2(T^*)^{3/2}]\exp(-p/T^*), \quad (80)$$

where

$$d_1=\frac{1-\gamma}{\tilde{\gamma}^2-1}\{\tfrac{1}{8}\pi p(\tilde{\gamma}^2-1)\}^{-1/2}\left\{1-\frac{\tilde{\gamma}^3 p}{\gamma+\tilde{\gamma}(1-p)}\right\},$$

$$d_2=\frac{1}{2}\frac{1-\gamma}{p(\tilde{\gamma}^2-1)}\{\tfrac{1}{8}\pi p(\tilde{\gamma}^2-1)\}^{-1/2}\left\{1+\frac{\tilde{\gamma}^3 p}{\gamma+\tilde{\gamma}(1-p)}\right\}, \quad (81)$$

$$F_{\mathrm{trial}}/JN=E_{\mathrm{trial}}-[\tfrac{1}{8}\pi p(\tilde{\gamma}^2-1)]^{-1/2}(T^*)^{3/2}\times\exp(-p/T^*). \quad (82)$$

The p and $\tilde{\gamma}$ that occur in Eqs. (75)–(83) refer to their zero-temperature values.

6. HIGH-TEMPERATURE LIMIT

For large T^*, the thermodynamic functions can be expanded in powers of $(T^*)^{-1}$. When this is done, the following expressions are obtained for p and $\tilde{\gamma}$ to first order in $(T^*)^{-1}$:

$$p=1-\tfrac{1}{4}(1-\gamma)(T^*)^{-1}; \quad \tilde{\gamma}=\gamma\{1+\tfrac{1}{2}(1-\gamma)(T^*)^{-1}\}. \quad (83)$$

Katsura and Inawashiro[14] give the exact expansion of the partition function. To order $(T^*)^{-2}$ it is

$$N^{-1}\ln(2^{-N}Z)=\tfrac{1}{2}\{[(1+\gamma)/4]^2(T^*)^{-2}+2[(1-\gamma)/4]^2(T^*)^{-2}\}. \quad (84)$$

The variational partition function is

$$N^{-1}\ln(2^{-N}Z_{\mathrm{trial}})=\tfrac{1}{16}(1+\gamma^2)(T^*)^{-2}. \quad (85)$$

The variational partition function at high temperature is close to the exact partition function only in the neighborhood of $\gamma=1$, the Ising limit.

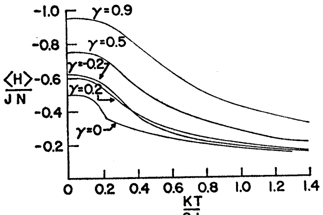

FIG. 5. Internal energy of the ferromagnet as a function of temperature for various values of anisotropy.

[14] S. Katsura and S. Inawashiro, J. Math. Phys. **5**, 1103 (1964).

7. INTERMEDIATE TEMPERATURES

First we consider the isotropic antiferromagnet and ferromagnet. In this limit, the variational equations are

$$\tilde{\gamma}\left[1-2\pi^{-1}\int_0^{\pi/2}dk\,\Lambda_k^{-1}\tanh\left(\frac{p}{2T^*}\Lambda_k\right)\right]=0, \quad (86)$$

$$-(1-p)+2\pi^{-1}\int_0^{\pi/2}dk\,\cos^2k\,\Lambda_k^{-1}\tanh\left(\frac{p}{2T^*}\Lambda_k\right)=0. \quad (87)$$

The above two equations have two sets of solutions:

$$\tilde{\gamma}=0, \quad (88)$$

$$-(1-p)+2\pi^{-1}\int_0^{\pi/2}dk\,\cos k\,\tanh\left(\frac{p}{2T^*}\Lambda_k\right)=0, \quad (89)$$

and

$$1-2\pi^{-1}\int_0^{\pi/2}dk\,\Lambda_k^{-1}\tanh\left(\frac{p}{2T^*}\Lambda_k\right)=0, \quad (90)$$

$$-(1-p)+2\pi^{-1}\int_0^{\pi/2}dk\,\cos^2k\,\Lambda_k^{-1}\tanh\left(\frac{p}{2T^*}\Lambda_k\right)=0. \quad (91)$$

For T^* negative, (90) can never be satisfied. Therefore, the variational equations for the isotropic antiferromagnet are (89) and (90). This is exactly Bulaevskii's result.[15] He gives the following high- and low-temperature expansion for p.

$$p=(1+2\pi^{-1})-\frac{\pi}{3[1+(2/\pi)]^2}(T^*)^2 \qquad T^*\ll 1, \quad (92)$$

$$p=1+\tfrac{1}{4}\,|T^*|^{-1} \qquad T^*\gg 1. \quad (93)$$

Now consider the isotropic ferromagnet. In the limit of zero temperature, the two solutions of (90) and (91), $\tilde{\gamma}=\pm 1$ with $p=\frac{1}{2}$, give the exact ground-state energy. However, there exists a temperature T_0^* above which these equations cannot be satisfied. A numerical calculation yields $T_0^*=0.2262$ with $\tilde{\gamma}=0$ and $p=0.54572$. Above T_0^* (88) and (89) minimize the free energy and at $T^*=T_0^*$ both sets of equations give the same value for F_{trial}. Figure 4, a plot of $\tilde{\gamma}$ versus T^* for various values of the anisotropy parameter, shows that in the isotropic limit $\tilde{\gamma}$ changes from ± 1 to 0 over a small temperature range. In fact it can be shown that

$$\lim_{T^*\to T_0^*}(d\tilde{\gamma}/dT^*)\to\pm\infty.$$

The internal energy is continuous but has a cusp at $T^*=T_0^*$. The specific heat, the derivative of the internal energy with respect to T^*, is discontinuous at T_0^* with the specific heat on the high-temperature side being less than that on the low-temperature side. This behavior corresponds to a second-order phase transition

[15] L. N. Bulaevskii, Zh. Eksperim. i Teor. Fiz. **43**, 968 (1962) [English transl.: Soviet Phys.—JETP **16**, 685 (1963)].

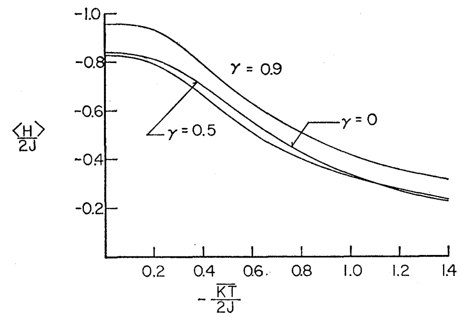

FIG. 6. The antiferromagnet's internal energy versus temperature for various values of anisotropy.

for which the trial Hamiltonian has gone from the Ising to the isotropic XY model. A measure of the short-range order of the system is given by $\partial F_{\text{trial}}/\partial\gamma$. This quantity is discontinuous as a function of γ at $\gamma=0$ for $T^*<T_0^*$, because of the two solutions of (90). However for $T^*>T_0^*$, the variational equations have only one solution and the short-range order is a continuous function of γ.

The solution of Eqs. (45) and (46) for all values of anisotropy, γ, and exchange constant, J, shows that all the thermodynamic functions are well behaved except in the aforementioned case of the isotropic ferromagnet. The results of these calculations are shown in Figs. (5) through (8), where Figs. (5) and (6) are the internal energies and Figs. (7) and (8) are the specific heats of the ferromagnet and antiferromagnet.

8. DISCUSSION AND CONCLUSIONS

In this paper we have found an upper bound to the free energy of the anisotropic Heisenberg magnet by means of the Bogolyubov variational principle. This investigation showed that the thermodynamic functions of the antiferromagnet as well as for the ferromagnet with $\gamma\neq 0$, are smooth, and well behaved, for all values of anisotropy, the isotropic antiferromagnetic case agreeing with the work of Katsura[3] and Bulaevskii.[15] In the zero-temperature limit, the variational ground-state energy was found to be in good agreement with the exact results.

The isotropic ferromagnet has a discontinuity in the specific heat at a temperature T_0^*, this behavior fitting Ehrenfest's criteria of a second-order phase transition. We attribute the phase transition to the discontinuous nature of the short-range as a function of γ below T_0^*, the discontinuity disappearing above T_0^*. Katsura's model[16] of the isotropic ferromagnet also shows a discontinuity in the specific heat analogous to that of ours.

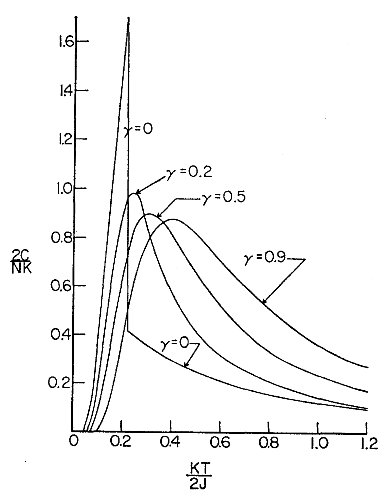

FIG. 7. Ferromagnetic specific heat in units of $2/NK$, as a function of temperature for various values of anisotropy.

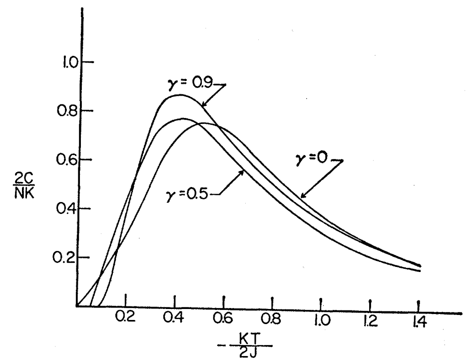

FIG. 8. Antiferromagnetic specific heat, in units of $2/NK$, versus temperature for various values of anisotropy.

To give a better physical explanation of this phase transition, one would like to calculate the longitudinal magnetic susceptibility or the long-range order. However there is no simple means by which the magnetic susceptibility can be calculated in the X–Y plane. This difficulty arises from the fact the total spin along the X or Y axis cannot be expressed in a simple quadratic form of Fermi operators, due to the nonlinear nature of the Jordan-Wigner transformation. Lieb, Schultz, and Mattis show that the long-range order for the XY model is zero at all finite temperatures. But the XY model is equivalent to a system of noninteracting fermions, whereas the Heisenberg model has interactions via the Z component of spins. It is just these interactions, however, that make the computation of the long-range order intractable.

[16] S. Katsura and S. Inwashiro, J. Math. Phys. 6, 1916 (1965).