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Rigorous and Spin-Wave-Type Results for the Lattice of Plane Rotors*

J. D. Patterson† and G. L. Jones
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
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The lattice of plane rotors which we have considered consists of two-dimensional spins on a two-dimensional lattice. While it is an intrinsically classical system, it shows many of the features of models which more realistically describe magnetic systems coupled in two-dimensional arrays. We start with the static properties and show how to derive generalizations of the theorems of Mermin and Wagner, and Jasnow and Fisher. The latter theorems require that the spontaneous magnetization vanish for two-dimensional Heisenberg systems. We consider more general interactions between spins than that implied by the Heisenberg model. We also note that higher moments of the magnetization must vanish as well. We derive explicit upper bounds on the mean-square magnetization when anisotropy is present. As an aid to visualization, we propose a dynamics for the lattice of plane rotors. We construct the dynamics in such a way as to leave the static statistical properties unaffected. A spin-wave-like approximation in this dynamics reduces the problem to a typical small-oscillations problem. We show (both rigorously and in the spin-wave-like approximation) that the qualitative effects of anisotropies and fields in a preferred direction are the same for certain properties.

I. INTRODUCTION

The properties of two-dimensional magnetic systems have been the subject of several experimental[1,2] as well as theoretical papers.[3–6] Two-dimensional Ising systems (without an external magnetic field) are well understood[7] and will not be discussed here. Most of the crystals whose magnetic properties are described by planar couplings of spins seem to be Heisenberg-like. We will therefore concentrate on Heisenberg systems. Isotropically coupled systems appear to be the simplest to analyze. However, we discuss some of the effects of anisotropy, because this will be present in any real crystal. The two-dimensional magnetic behavior of actual crystals manifests itself most clearly at low temperatures. The only widely used technique for calculating the properties of magnetic systems at low temperatures is the method of spin waves (or an equivalent approximation). Due to the fact that the magnetization vanishes for two-dimensional (2D) isotropic Heisenberg systems our approach to spin-wave theory, which is based on the existence of an ordered ground state, is not consistent for this situation.[8] However, for sufficiently large external fields and/or suitable anisotropies, our method of discussing spin waves is a good method even in two dimensions. Thus, we find it useful to include a discussion of a spin-wave-like approximation in two dimensions.

Our aim is to discuss some of the features of two-dimensional magnetic systems in as simple a fashion as possible, and we have chosen the lattice of plane rotors[9] as the simplest system. In this model the spins are considered to be two dimensional, and so they must be treated classically. Fortunately, the behavior of classically interacting spins still appears to show most of the properties of actual magnetic systems[10] although the precise temperature dependences of quantities of interest may be different for the classical case than the quantum case. With a Heisenberg-type coupling between spins (and no kinetic energy terms) we can discuss the static magnetic properties. We can (in the same model) make a spin-wave-like approximation and calculate the static magnetic properties at low temperatures. With no kinetic energy terms, however, our system has no inherent dynamics, and it is not possible to picture in a dynamical fashion what we mean by a spin-wave-like approximation (for two-dimensional spins one cannot have true spin waves because precession is impossible). This is rather unsatisfying, but fortunately we are free to enlarge our model in such a way that the new model has a dynamics and also has the same static magnetic properties as the old model. In our new model, we can picture spin-wave-like properties as well as calculate them. The new model shows how the spin-wave-like approximation can be regarded as equivalent to the small-oscillation theory of classical mechanics. Finally, we should mention that the isotropic lattice of plane rotors with purely Heisenberg coupling is also sometimes called the Vaks-Larkin[11] model, and for a three-dimensional lattice it has been suggested as a model to describe the superfluid transition in a Bose fluid.

II. LATTICE OF CLASSICAL PLANE ROTORS

We assume a square array of spins all with length $|\vec{S}_i| = S$, lying in the x-y plane. We assume the spin located at $\vec{R}_i$ is inclined at an angle θ_i with the horizontal x axis. With an external field B (in suitable units) along the x axis, we assume the coupling between all N spins can be described by the following Hamiltonian:

$$H=-\sum_{i,j=1}^{N}\{f[J(\vec{R}_i-\vec{R}_j)\vec{S}_i\cdot\vec{S}_j] +a(\vec{R}_i-\vec{R}_j)S_{ix}S_{jx}\}-B\sum_{i=1}^{N}S_{ix} \quad . \qquad (1)$$

The $J(\vec{R}_i-\vec{R}_j)$, often called the exchange integrals, measure the strength of coupling between the pairs of spins i and j. The anisotropy term is determined by $a(\vec{R}_i-\vec{R}_j)$. We assume both J and a are of finite range, that $J(0)=a(0)=0$, and that $f(0)=0$. We assume only ferromagnetic interactions so that $J\geq 0$. We also assume f satisfies $f'(x+\epsilon)\geq f'(x)$ and $f''(x+\epsilon)\geq f''(x)$ for $\epsilon>0$. For example, $f(x)=x+x^2$ would satisfy all our requirements and include the physically interesting case of the Heisenberg Hamiltonian modified by a biquadratic interaction. If $f(x)=x$ and $a=0$, then our model describes an isotropic Heisenberg system placed in an external field.

Using the angles θ_i, we can also write our model Hamiltonian as

$$H=-\sum_{i,j=1}^{N}\{f[S^2J(\vec{R}_i-\vec{R}_j)\cos(\theta_i-\theta_j)] +a(\vec{R}_i-\vec{R}_j)S^2\cos\theta_i\cos\theta_j\}-B\sum_{i=1}^{N}S\cos\theta_i . \qquad (2)$$

In this notation, the magnetization can be written

$$m_x=\sum_{i=1}^{N}\frac{S}{N}\cos\theta_i \quad . \qquad (3)$$

Note that the Zeeman energy in (2) can also be written $-NBm_x$. We will assume periodic boundary so that all quantities such as m_x and H repeat themselves outside the basic crystal.

When we take thermodynamic measurements, we do not actually measure m_x and H but rather their statistical average, $\langle m_x\rangle$ and $\langle H\rangle$. We can calculate these averages by the standard techniques of statistical mechanics. For a canonical ensemble and for systems of interest to us, we know for arbitrary $f=f(\theta_1\cdots\theta_N)$:

$$\langle f\rangle=\int_\Gamma e^{-\beta H}f(\theta_1\cdots\theta_N)\,d\Gamma\Big/\int_\Gamma e^{-\beta H}\,d\Gamma \quad , \qquad (4)$$

where $d\Gamma=\prod_{i=1}^{N}d\theta_i$, $\beta=1/(k_BT)$, T is the temperature in K, and k_B is Boltzmann's gas constant.

III. RIGOROUS THEOREMS

We follow several authors[12–14] in using Schwarz inequalities to derive rigorous inequalities. The Schwarz inequalities depend only on very general properties of vector spaces and one can show that

$$\langle A^*A\rangle\langle B^*B\rangle\geq|\langle A^*B\rangle|^2 \quad , \qquad (5)$$

for the inner product $\langle A^*A\rangle$ defined in such a way as to give the statistical average of A^*A.

The main topic of this section is to use Eq. (5) to produce upper bounds for $\langle m_x^2\rangle$. Some preliminary details are necessary, however. Let

$$A_{\vec{k}}=\sum_{i=1}^{N}e^{i\vec{k}\cdot\vec{R}_i}\frac{S}{N}\sin\theta_i \qquad (6)$$

and

$$B_{\vec{k}}=\sum_{j=1}^{N}e^{i\vec{k}\cdot\vec{R}_j}e^{\beta H}\left(\frac{\partial}{\partial\theta_j}e^{-\beta H}G\right) \quad , \qquad (7)$$

where G is real (its form will be chosen later). The $\vec{k}$ vectors are the usual wave vectors defined in reciprocal space and they range over the first Brillouin zone (BZ).

An upper bound for $\sum_{\vec{k}}\langle A_{\vec{k}}^*A_{\vec{k}}\rangle$ is readily obtained:

$$\sum_{\vec{k}(BZ)}\langle A_{\vec{k}}^*A_{\vec{k}}\rangle=(S^2/N)\sum_i\langle\sin^2\theta_i\rangle\leq S^2 \quad . \qquad (8)$$

By a partial integration on θ_j, we can show that

$$\langle A_{\vec{k}}^*B_{\vec{k}}\rangle=-\langle Gm_x\rangle \quad . \qquad (9)$$

Finally, we can obtain a useful upper bound on $\langle B_{\vec{k}}^*B_{\vec{k}}\rangle$.

By two partial integrations we find

$$\langle B_{\vec{k}}^*B_{\vec{k}}\rangle=\sum_{i,j=1}^{N}e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)}\left\langle\frac{\partial G}{\partial\theta_i}\frac{\partial G}{\partial\theta_j}+\beta G^2\frac{\partial^2H}{\partial\theta_i\partial\theta_j}\right\rangle, \qquad (10)$$

where the Hamiltonian is defined by Eq. (2). By substituting the expression for

$$\frac{\partial^2H}{\partial\theta_i\partial\theta_j} \quad ,$$

and by defining

$$\Omega=\sum_iR_i^2\left[|f'(S^2J(\vec{R}_i))||J(\vec{R}_i)| +|f''(S^2J(\vec{R}_i))|S^2|J(\vec{R}_i)|^2\right] \quad , \qquad (11)$$

$$\Omega_a=\sum_i|a(\vec{R}_i)| \quad , \qquad (12)$$

we can say

$$\langle B_{\vec{k}}^*B_{\vec{k}}\rangle\leq\sum_{i,j=1}^{N}\left|\left\langle\frac{\partial G}{\partial\theta_i}\frac{\partial G}{\partial\theta_j}\right\rangle\right|+N\beta S^2\,\Omega\langle G^2\rangle k^2 +N\beta S|B|\langle G^2\rangle+4N\beta S^2(\Omega_a)\langle G^2\rangle \quad , \qquad (13)$$

where in deriving this inequality use has been made of the assumptions that f' and f'' are nondecreasing.

Combining Eqs. (5), (8), (9), and (13), we can write, with $G=m_x$,

$$S^2\geq N\frac{\rho}{(2\pi)^2}\int_0^{k_0}\frac{2\pi k\,dk}{S^2+N\beta S^2\langle m_x^2\rangle[\Omega k^2+|B|/S+4(\Omega_a)]}\times|\langle m_x^2\rangle|^2 \quad , \qquad (14)$$

where $k_0>0$ but smaller than $\frac{1}{2}$|(smallest reciprocal-lattice vector)|. In deriving (14), we have used the fact that for 2D systems and large N,

$$\sum_{\vec{k}}(\;)\to N\frac{\rho}{(2\pi)^2}\int(\;)\,d\vec{k} \quad ,$$

where $\rho = A/N \to$ constant as N, $A \to \infty$, and A denotes area. There are two interesting limits in which (14) can be evaluated. Consider first the case that $|B| = (\Omega_a) = 0$, and suppose N is large. We find

$$\langle m_x^2 \rangle \leq (4\pi S^4 \Omega/\rho)\, \beta\, (1/\ln N) \to 0 \quad \text{as } N \to \infty \quad . \qquad (15)$$

Equation (15) is consistent with, but more general (it includes more general sorts of isotropic interactions) than, the quantum-mechanical result stated by Jasnow and Fisher.[5] If one is doing numerical studies on finite systems, (15) might also be useful for finite but large N.

The other interesting limit in which (14) can be evaluated is when we let $N \to \infty$ right away and assume small anisotropies and fields. We then find

$$\langle m_x^2 \rangle \leq (4\pi S^4 \Omega/\rho)\, \beta / \left| \ln(|B| + 4(\Omega_a) S) \right|$$

$$\to 0 \qquad \text{as } |B| + 4S(\Omega_a) \to 0 \quad . \qquad (16)$$

This is consistent with the result of Mermin and Wagner[3] and Mermin[9] [who find $\langle m_x \rangle < K(|\ln|B||)^{-1/2}$, where K is a constant with no anisotropy and for purely Heisenberg interactions] since we believe $\langle m_x^2 \rangle = \langle m_x \rangle^2$ in the thermodynamic limit. This does not imply that $\chi = 0$. It is even possible for $\langle m_x^2 \rangle - \langle m_x \rangle^2$ to be zero as $N \to \infty$ and for χ to diverge in the same limit. This would happen if, for example, $\langle m_x^2 \rangle - \langle m_x \rangle^2 \propto (\ln N)^{-1}$. Mermin obtains the classical result, whereas Mermin and Wagner's result is derived quantum mechanically.

We could similarly rule out spontaneous magnetization for one-dimensional systems simply by integrating over one-dimensional k space. An integration over three-dimensional $\vec{k}$ space yields the expected result that $\langle m_x^2 \rangle$ is not required to vanish.

We could also establish (by different choices of G and induction) that all even moments should vanish (with no anisotropy or fields). [A bound on $\langle m_x^4 \rangle$, for example, can be obtained by letting $G = m_x^3$ and then doing a calculation similar to the calculation that was done in deriving Eq. (15).] We shall not do this because intuitively we expect in the thermodynamic limit that, e.g., $\langle m_x^4 \rangle = \langle m_x^2 \rangle^2$, and we have already established that $\langle m_x^2 \rangle = 0$.

We could also show by a somewhat different argument based on the Schwarz inequalities, that the transverse susceptibility is infinite for the isotropic system in the limit of vanishing field.[13] This is also intuitive because all it means is that it takes no energy to rotate a magnetic moment in an isotropic system.

Finally, we should note that these theorems do not rule out all kinds of phase transitions. In particular the appearance of infinite magnetic susceptibility without the appearance of spontaneous magnetization is a possibility for isotropic 2D Heisenberg systems.[4,5,9]

IV. SPIN-WAVE THEORY

We enlarge our Hamiltonian by adding a kinetic energy term so that dynamical motion will be possible. As mentioned, this is not necessary in order to calculate those properties of interest to us, but it is convenient for visualization purposes. Wegner[9] has obtained similar results to those given below. Our results are more general in that they include more general exchange interactions than implied by the Heisenberg model and also we include anisotropy. Also, Wegner does not introduce a dynamics. We say (introducing a constant α)

$$H^1 = \sum_{i=1}^{N} (p_i^2/2\alpha) + H \qquad (17)$$

will describe the motion of the system, where H is defined by Eq. (2) and $p_i = \alpha\dot{\theta}$. Note that statistical averages for quantities that are functions of θ_i (and not p_i) are invariant to adding in the kinetic energy term. For our model the spin-wave-like approximation consists in treating θ_i as small and retaining only terms up to second order in θ_i in the Hamiltonian. If the x direction is the ordering direction, this is consistent with the typical spin-wave approximation of assuming $S_y \ll S_x$.[15]

Our Hamiltonian generates a typical small-oscillation problem and the normal frequencies obtained are

$$\omega_k^2 = \frac{S^2 f_F(0)}{\alpha} \left(2 - \cos k_x a - \cos k_y a + \frac{2a_F(0) + B/S}{f_F(0)} \right) , \qquad (18)$$

where

$$f_F(0) = \textstyle\sum_i f'(S^2 J(\vec{R}_i)) J(\vec{R}_i)$$

and

$$a_F(0) = \textstyle\sum_i a(R_i) \quad .$$

We now indicate how to calculate the magnetization. Consistent with the spin-wave approximation, we can say

$$\langle m_x \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle S_{x,i} \rangle = \frac{S}{N} \sum_{i=1}^{N} \langle \cos\theta_i \rangle$$

$$\cong S\left(1 - \frac{1}{2N} \sum_{i=1}^{N} \langle \theta_i^2 \rangle \right) \quad . \qquad (19)$$

The remaining problem is the problem of evaluating

$$\frac{1}{N} \sum_{i=1}^{N} \langle \theta_i^2 \rangle \quad .$$

By using normal coordinates $\Delta_{\vec{k}}$ in the usual way, we can readily show that the energy E of the system described by the Hamiltonian H^1 is

$$E = \frac{\alpha}{2} \sum_{\vec{k}\,(\mathrm{BZ})} (\dot{\Delta}_{\vec{k}} \dot{\Delta}_{\vec{k}}^* + \omega_{\vec{k}}^2 \Delta_{\vec{k}} \Delta_{\vec{k}}^*) \quad . \qquad (20)$$

Writing E in terms of $\Delta_{\vec{k}}$ corresponds to using "running waves" as solutions. The $\Delta_{\vec{k}}$ are slightly inconvenient because the $\Delta_{\vec{k}}$ and $\Delta_{-\vec{k}}$ modes are still coupled in (20). It is possible to make a transformation to "standing wave" modes described by *real* $C_{\vec{k}}$ with the same frequency $\omega_{\vec{k}}$ so that E may be expressed as in (20) but with the $\Delta_{\vec{k}}$ replaced by $C_{\vec{k}}$.[16] The problem is now explicitly reduced to a set of N decoupled harmonic oscillators. We obtain for the magnetization (since $\sum_{i=1}^{N}\theta_i^2=\sum_{\vec{k}'}|\Delta_{k'}|^2=\sum_{\vec{k}'}C_{\vec{k}'}^2$) by (19)

$$\langle m_x\rangle = S\left[1-\frac{1}{2N}\sum_{\vec{k}'}\frac{\int e^{-\beta E}C_{\vec{k}'}^2(\prod_{BZ}d\dot{C}_{\vec{k}})(\prod_{BZ}dC_{\vec{k}})}{\int e^{-\beta E}(\prod_{BZ}d\dot{C}_{\vec{k}})(\prod_{BZ}dC_{\vec{k}})}\right]. \tag{21}$$

We are only interested in the low-temperature results, so large amplitudes and velocities should appear with vanishingly small probability. Therefore, we can safely extend the upper limits of the integrals to ∞. With $\Delta_{\vec{k}}$ replaced by $C_{\vec{k}}$ we insert (20) into (21), cancel common factors in the numerator and denominator, evaluate standard integrals, and replace the sum over the BZ by an integral. We are only interested in low temperatures and so only large wavelength (small $|\vec{k}|$) modes should be of importance. Finally, at low temperatures the shape of the BZ should not be important so we can use as an upper limit for our integral k_μ defined by $\pi k_\mu^2=(2\pi/a)^2$ where a is the nearest-neighbor distance. We thus obtain for our two-dimensional systems:

$$\langle m_x\rangle = S\left[1-\frac{1}{\beta}\frac{\rho}{4\pi}\frac{1}{S^2 f_F(0)a^2}\times\ln\left(1+\frac{f_F(0)a^2k_\mu^2}{2(2a_F(0)+B/S)}\right)\right]. \tag{22}$$

Note that if no anisotropies or fields are present $[a_F(0)=B=0]$ then (22) diverges and our spin-wave approximation is inappropriate. This fact was known before Mermin and Wagner proved the magnetization must vanish for this case.

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Paramagnetic and Antiferromagnetic Phases in the Half-Filled Narrow Energy Band*

Laurent G. Caron† and G. Kemeny‡
Department of Electrical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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The effect of correlation on the antiferromagnetic and paramagnetic phases of Hubbard's model of a half-filled narrow band are investigated using second-order perturbation theory. Employing the gap of the antiferromagnetic state as a variational parameter, it is shown that the increase of the bandwidth/potential-energy ratio leads to a phase transition into the paramagnetic state nearly where Mott has estimated it to occur. The convergence of the perturbation expansion is shown to be excellent at the transition.

I. INTRODUCTION

In a recent paper[1] the authors discussed the mathematical methods they believed necessary for the treatment of the paramagnetic and antiferromagnetic ranges of the Hubbard Hamiltonian[2] in a half-filled narrow band. They argued that a t-matrix expansion would be required in the investi-