

EXACT RESULTS FOR THE ONE-DIMENSIONAL, ANISOTROPIC CLASSICAL HEISENBERG MODEL*

Wheatstone Physics Laboratory, King's College, London, England
(Received 24 July 1967)

We obtain the zero-field partition function and correlation functions of the one-dimensional, anisotropic classical Heisenberg model exactly and find similar results for an anisotropic "planar" spin model. The isotropic and the anisotropic cases have greatly different low-temperature behavior.

Although the one-dimensional, spin- $\frac{1}{2}$, anisotropic Heisenberg model has been intensively studied, the partition function and correlation functions of the model have not yet been obtained exactly for general anisotropy and temperatures. In this Letter it is shown that such results can be simply derived for the anisotropic classical Heisenberg model.

The Hamiltonian for the classical model is written as

$$\mathcal{H} = - \sum_{i=1}^N 2J_{\parallel} \times [s_{iz} s_{i+1z} + \tanh\mu (s_{ix} s_{i+1x} + s_{iy} s_{i+1y})], \quad (1)$$

where $s_{ix} = \sin\theta_i \cos\varphi_i$, $s_{iy} = \sin\theta_i \sin\varphi_i$, $s_{iz} = \cos\theta_i$, $\tanh\mu = J_{\perp}/J_{\parallel} \equiv \gamma$, $\mu \geq 0$, and $s_{N+1} \equiv s_1$ (corresponding to cyclic boundary conditions). Following the method¹ used to evaluate the partition function of the isotropic model, we can write the partition function of a ring of N anisotropic spins as

$$Z_N = \sum_{l=0}^{\infty} \sum_{m=-l}^l \lambda_{ml}^N, \quad (2)$$

where λ_{ml} are the eigenvalues of the integral equation

$$\int_{\Omega_2} C(\theta_1, \varphi_1, \theta_2, \varphi_2) \Psi_{ml}(\theta_2, \varphi_2) d\Omega_2 / 4\pi = \lambda_{ml} \Psi_{ml}(\theta_1, \varphi_1), \quad (3)$$

and $d\Omega_2$ is the element of solid angle $\sin\theta_2 d\theta_2 d\varphi_2$. The kernel of Eq. (3) is

$$C(\theta_1, \varphi_1, \theta_2, \varphi_2) = \exp K [s_{1z} s_{2z} + \tanh\mu (s_{1x} s_{2x} + s_{1y} s_{2y})], \quad (4)$$

where $K = 2J_{\parallel}/kT$. It may be readily shown that the normalized eigenfunctions are the angle spheroidal wave functions²

$$\Psi_{ml}(\theta, \varphi) = 2^{\frac{1}{2}} \Lambda_{|m|l}^{-\frac{1}{2}}(h) S_{|m|l}(h, \cos\theta) e^{im\varphi}, \quad (5)$$

where $h = -iK/\cosh\mu$, $l = 0, 1, 2, \dots$, and $|m| \leq l$. The corresponding eigenvalues are the radial functions²

$$\lambda_{ml} = i^l j_e{}_{|m|l}(h, \cosh\mu). \quad (6)$$

In the thermodynamic limit, only the largest eigenvalue contributes to Eq. (2). Thus

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N = \ln [j_e{}_{00}(h, \cosh\mu)]. \quad (7)$$

This expression reduces, in the limit $\mu \rightarrow \infty$, to $\ln(K^{-1} \sinh K)$ in agreement with previous results.^{1,3} For the classical Ising model ($\mu = 0$) we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N = \ln [j_e{}_{00}(-iK, 1)]. \quad (8)$$

A high temperature series for the partition function (7) and a perturbation series about the isotropic result in powers of $1-\gamma^2$ can both be derived from the standard expansion of the radial function in terms of modified Bessel functions.⁴ The low-temperature asymptotic expansion for the energy per spin of the classical Ising model is

$$(E/2J_{\parallel}) \sim -1 + K^{-1} + \frac{1}{4}K^{-2} + \frac{7}{48}K^{-3} + \dots \quad (9)$$

This result is simply obtained from the formulas given by Sips.⁵ At low temperatures the behavior of the specific heat of the classical Ising model differs considerably from that of the isotropic model.³

The zero-field spin-spin correlation functions can also be calculated in terms of the eigenfunctions (5) and eigenvalues (6). The final results (for N large) are given below:

$$\langle s_{iz} s_{jz} \rangle = \sum_{l \text{ odd}} (\lambda_{0l}/\lambda_{00})^{|i-j|} D_l(h), \quad (10)$$

$$\begin{aligned} \langle s_{ix} s_{jx} \rangle &= \langle s_{iy} s_{jy} \rangle \\ &= \frac{1}{2} \sum_{l \text{ odd}} (\lambda_{1l}/\lambda_{00})^{|i-j|} E_l(h), \end{aligned} \quad (11)$$

where

$$D_l(h) = \Lambda_{00}^{-1} \Lambda_{0l}^{-1} \left[\int_{-1}^1 S_{00}(h, \eta) S_{0l}(h, \eta) \eta d\eta \right]^2, \quad (12)$$

$$E_2(h) = \Lambda_{00}^{-1} \Lambda_{1l}^{-1} \times \left[\int_{-1}^1 S_{00}(h, \eta) S_{1l}(h, \eta) (1 - \eta^2)^{1/2} d\eta \right]^2, \quad (13)$$

and $i \neq j$. The self-correlation function ($i = j$) are

$$\langle (s_{iz})^2 \rangle = \frac{1}{3} + \frac{2}{3} F(h), \quad (14)$$

$$\langle (s_{ix})^2 \rangle = \langle (s_{iy})^2 \rangle = \frac{1}{3} - \frac{1}{3} F(h), \quad (15)$$

where

$$F(h) = \Lambda_{00}^{-1} \int_{-1}^1 P_2(\eta) S_{00}^2(h_1, \eta) d\eta, \quad (16)$$

and $P_2(\eta)$ is the Legendre polynomial of order 2. It follows immediately from Eq. (16) that $F(h)$ satisfies the inequality $-\frac{1}{2} \leq F(h) \leq 1$. [In the isotropic limit $F(h) = 0$.] For large $|i-j|$ and $T > 0$ the correlations (10) and (11) decay exponentially.

Using fluctuation relations, the zero-field parallel susceptibility is found from the correlation functions (10) and (14) and the perpendicular susceptibility from the correlation functions (11) and (15). The nature of the divergence in $kT\chi_{\parallel}$ at low temperatures is determined by the behavior of $\lambda_{01}/\lambda_{00} - \lambda_{01}$. It is found⁶ that λ_{01} and λ_{00} have the same asymptotic expansions as $T \rightarrow 0$ for $0 \leq \gamma < 1$. Thus $kT\chi_{\parallel}$ has an exponential-like divergence for $0 \leq \gamma < 1$. For the isotropic case $kT\chi_{\parallel} \sim 1/T$.

The eigenfunctions and eigenvalues for $\mu < 0$ are exactly similar to (5) and (6) except that Eq. (6) has a factor of $(-1)^m$. It is interesting to note that the case $\gamma = -\frac{1}{2}$ provides a solution for the "nearest-neighbor" dipole-dipole interaction in one dimension. Antiferromagnetic properties are obtained by putting K equal to $-|K|$.

In order to extend the range of anisotropy, it is convenient to define the Hamiltonian

$$\mathcal{H} = - \sum_{i=1}^N 2J_{\perp} [\tanh \rho s_{iz} s_{i+1x} + (s_{ix} s_{i+1x} + s_{iy} s_{i+1y})], \quad (17)$$

where $\tanh \rho = J_{\parallel}/J_{\perp}$. For this model the eigenfunctions are the same as in Eq. (5), with $h = K/\cosh \rho$ and $K = 2J_{\perp}/kT$. The eigenvalues

are

$$\lambda_{ml} = i^l j e_{|m|l}(h, -i \sinh \rho). \quad (18)$$

Hence, the partition function for N large is given by

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N = \ln [j e_{00}(h, -i \sinh \rho)], \quad (19)$$

while the correlation functions are formally the same as Eqs. (10), (11), (14), and (15). The low-temperature expansion for the energy of the transverse model ($\rho = 0$) is⁷

$$(E/2J_{\perp}) \sim -1 + K^{-1} + \frac{1}{4} K^{-2} + \frac{23}{64} K^{-3} + \dots \quad (20)$$

The divergence of $kT\chi_{\perp}$ as $T \rightarrow 0$ is determined by the behavior of $\lambda_{11}/\lambda_{00} - \lambda_{11}$. It is found that⁷ when $\rho = 0$, $kT\chi_{\perp} \sim 1/T$ as $T \rightarrow 0$.

Similar results can be derived for the anisotropic, "planar," classical Heisenberg model with a Hamiltonian

$$\mathcal{H} = - \sum_{i=1}^N 2J_x [s_{ix} s_{i+1z} + \tanh \xi s_{iy} s_{i+1y}], \quad (21)$$

where $s_{ix} = \cos \varphi_i$ and $s_{iy} = \sin \varphi_i$ are components of a two-dimensional unit vector, $\tanh \xi = J_y/J_x \equiv \gamma$, $\xi \geq 0$. The eigenfunctions for this model are the Mathieu functions⁸ $ce_m(\varphi, -h^2)$ and $se_{m+1}(\varphi, -h^2)$, while the corresponding eigenvalues are the radial functions $i^m M c_m(1) \times (\xi, -ih)$ and $i^{m+1} M s_{m+1}(1)(\xi, -ih)$, where $m = 0, 1, 2, \dots$, $h = K/2 \cosh \xi$ and $K = 2J_x/kT$. In the thermodynamic limit,

$$\frac{1}{N} \ln Z_{N+M} c_0^{(1)}(\xi, -ih). \quad (22)$$

Expressions for the correlation functions, similar to those given above, can be readily found. For example,

$$\langle (s_{ix})^2 \rangle = 1 - \langle (s_{iy})^2 \rangle = \frac{1}{2} + \frac{1}{2\pi} \int_0^{2\pi} c e_0^2(\varphi, -h^2) \cos 2\varphi d\varphi. \quad (23)$$

The zero-field susceptibility $kT\chi_x$ (obtained from the correlation function $\langle s_{ix} s_{jx} \rangle$) has an exponential-like divergence as $T \rightarrow 0$ for $0 \leq \gamma < 1$. When $\gamma = 1$, $kT\chi_x \sim 1/T$.⁹ This behavior is exactly similar to that of $kT\chi_{\parallel}$ given above.

Although we have assumed cyclic boundary conditions, it is possible to derive the properties of a finite open chain of $N+1$ spins. A

more detailed numerical study of the classical anisotropic models is in progress.

*This research has been supported in part by the U. S. Army through its European Research Office.

¹G. S. Joyce, Phys. Rev. **155**, 478 (1967).

²The notation adopted for the spheroidal wave functions is that given in P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill Book Company, Inc., New York, 1953), Chap. 11.

³M. E. Fisher, Am. J. Phys. **32**, 343 (1964).

⁴See Ref. 2 for details of this expansion.

⁵R. Sips, Trans. Am. Math. Soc. **90**, 340 (1959).

⁶See in C. Flammer, Spheroidal Wave Functions (Stanford University Press, Stanford, California, 1957), Chap. 8.

⁷See Ref. 5.

⁸The notation used for the Mathieu functions is that of J. Meixner and F. W. Schäfer, Mathieusche Funktionen und Sphäroidfunktionen (Springer-Verlag, Berlin, 1954).

⁹It is incorrectly stated in Ref. 1, p. 486, that χ for the isotropic "planar" model diverges as $1/T$.

RANGE OF A STATIC SPIN PERTURBATION IN PALLADIUM

A. M. Clogston

Bell Telephone Laboratories, Murray Hill, New Jersey

(Received 21 June 1967)

The structure of the large magnetic moments associated with certain first-row transition-metal atoms dissolved in palladium continues to be of interest. These giant moments have been reported by Gerstenberg¹ for Mn, Fe, Co, and Ni dissolved in Pd, by Crangle² for Fe in Pd, and by Bozorth *et al.*³ for Co in Pd. The systematic variation of the size of the moment with electron concentration in the host has been studied by Clogston *et al.* for Fe in Pd-Rh and Pd-Ag alloys.⁴ Geballe *et al.* have studied the magnetic moment found when Fe is dissolved in Pd-Pt solid solutions.⁵ Recently Low and Holden have investigated by inelastic neutron scattering the distribution of magnetic moment in the solvent for Fe and Co dissolved in Pd.⁶

The following general picture has emerged from this work. At the site of each iron atom substitutionally present in the Pd lattice, there exists a magnetic moment of 3-4 μ_B . Surrounding this site, the Pd atoms are polarized for a distance of about 10 Å. The nearest-neighbor atoms to the iron impurity carry a moment of about 0.07 μ_B . This moment falls off exponentially with distance at such a rate that the total moment of the complex is about 10 μ_B . The giant moment thus consists of a rather small spin density spread out over many atoms surrounding the impurity.

In a metal the disturbance in electronic structure created by an impurity atom is generally of very short range, the first zero in the oscillating Ruderman-Kittel-Yosida range function coming approximately at $r/a = 0.36/\nu^{1/3}$ for a spherical Fermi surface containing ν

electron or hole states per atom. Here a is the lattice constant for a fcc metal. In a free-electron approximation this range can be considerably extended by the introduction of a short-range, momentum-independent interaction between the electrons.^{7,8} However, the modified range function can be made to agree with experiment only by assuming unrealistic values of ν or of the interaction strength.⁹

We wish to describe here the effect of considering not only the intra-atomic exchange interaction between electrons on the same atom but also important effects due to interatomic exchange between electrons on nearest-neighbor atoms. We shall assume that the principal response of Pd to a weak spin-dependent perturbation is confined to the heavy-hole band lying at point X in the Brillouin zone and containing approximately 0.18 hole states per atom.¹⁰

For simplicity we consider first the case of a band made up of nondegenerate atomic orbitals and write the Bloch functions in the form

$$\Psi_{\vec{k}}(\vec{r}) = N^{-1/2} \sum_a \exp(i\vec{k} \cdot \vec{r}_a) \theta(\vec{r} - \vec{r}_a). \quad (1)$$

The extension to the case of degenerate orbitals appropriate to Pd has two important effects which will be discussed later. The z component of spin on atom a is written

$$S_{\vec{q}}(a) = (1/N) \sum_{\vec{q}} \exp(-i\vec{q} \cdot \vec{r}_a) S_{\vec{q}}, \quad (2)$$

where in the representation given by Eq. (1) $S_{\vec{q}}$ has the form

$$S_{\vec{q}} = \sum_{\vec{k}, \vec{k}'} \delta_{\vec{k}', -\vec{k}, \vec{q} + \vec{k}} \frac{1}{2} [C_{\vec{k}, \uparrow}^* C_{\vec{k}, \uparrow} - C_{\vec{k}, \downarrow}^* C_{\vec{k}, \downarrow}]. \quad (3)$$