

where  $\theta$  is a unit step function and  $f(C)$  the distribution of particle capacitances. The conductance through a particle is proportional to the area of the particle which in turn is proportional to the capacitance. The other  $C$  factor in the second integral stems from our choice of a uniformly distributed  $V_D$ .

It is easy to adapt this model to account for the effect of the superconducting transition of the Sn particles. The main effects are to increase the activation energy by half the superconducting energy gap in the particle and to change the density of states. Calculations of the dynamical resistance-versus-voltage characteristic using Eq. (2) gives good agreement with the experiment. In Fig. 3 the dashed curve is calculated for  $T=0$  and with  $f(C)$  computed from the elec-

tron micrograph assuming disklike particles with a 15-Å-thick oxide layer on both sides and a dielectric constant of 10.

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<sup>1</sup>D. Shoenberg, Proc. Roy. Soc. (London), Ser. A 175, 49 (1940).

<sup>2</sup>F. Wright, Phys. Rev. 163, 420 (1967).

<sup>3</sup>D. Markowitz, Physics 3, 199 (1967).

<sup>4</sup>P. W. Anderson, J. Phys. Chem. Solids 11, 26 (1959).

<sup>5</sup>J. H. P. Watson, Phys. Rev. 148, 223 (1966).

<sup>6</sup>L. Y. L. Shen and J. M. Rowell, Phys. Rev. 165, 566 (1968).

<sup>7</sup>F. Mezei, Phys. Letters 25A, 534 (1967).

<sup>8</sup>A. F. G. Wyatt and D. J. Lythall, Phys. Letters 25A, 541 (1967).

### CRITICAL PROPERTIES OF THE XY MODEL\*

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The XY model of a quantum lattice fluid or a ferromagnet is studied by the method of exact high-temperature series expansion. Nine terms are obtained in the free-energy series and seven in the series for the square of the fluctuation in the long-range order. Analysis of these series yields the critical values  $kT_c/J=4.84\pm 0.06$ ,  $\gamma=1.00\pm 0.07$ , and  $\alpha=-0.20\pm 0.20$  for the fcc lattice.

The XY model of interacting spin- $\frac{1}{2}$  particles is characterized by the interaction Hamiltonian,

$$\begin{aligned} \mathcal{H}_0 &= -J \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_i a_j^\dagger) \\ &\equiv -J \sum_{\langle ij \rangle} (\sigma_{ix} \sigma_{jx} + \sigma_{iy} \sigma_{jy}), \end{aligned} \quad (1)$$

where the sum is over nearest-neighbor pairs of sites on a lattice and the  $\sigma$ 's are Pauli matrices. Like the Ising and Heisenberg models,<sup>1</sup> the XY model is a special case of the anisotropic Heisenberg model.

Matsubara and Matsuda<sup>2</sup> introduced in 1956 a lattice model for liquid helium which reduces to the XY model for a hard-core molecular-interaction potential. In that case  $J = \hbar^2 d / 4mq a^2$ , where  $d$  is the dimensionality of the lattice,  $m$  is the molecular mass,  $q$  the coordination number, and  $a$  the nearest-neighbor distance on the lattice. Matsubara and Matsuda were able to show that, even in the molecular-field approximation, the XY model is more successful than the ideal Bose gas in several respects in predicting properties of the  $\lambda$  transition.

The XY model may also be realized in certain magnetic insulators in which  $g_\perp \gg g_\parallel$  because of a strong crystalline field splitting the  $s_z = \pm \frac{1}{2}$  Kramers doublet below the other magnetic sub-states of an ion such as Gd. In particular,  $\text{Gd}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$  seems to be such a substance.<sup>3</sup>

The physical significance of the anisotropic Heisenberg model, both as a lattice gas and as a ferromagnet, has been discussed recently by Fisher<sup>4</sup> and Whitlock and Zilsel<sup>5</sup> without, however, their making very extensive calculations. On the other hand, Yang and Yang<sup>6</sup> have obtained a number of exact results concerning the energy of the anisotropic Heisenberg model. Exact high-temperature series expansion techniques have been applied over a range of anisotropy including the case of the XY model by Obokata, Ono, and Oguchi<sup>7</sup> and by Pirnie,<sup>8</sup> but their series have not been extended sufficiently far to obtain reliable information about the critical region.

A high-temperature expansion of the zero-field partition function,  $Z$ , can be obtained starting from the expression

$$Z = \text{tr} \{ 1 - \beta \mathcal{H}_0 + \beta^2 \mathcal{H}_0^2 / 2! - \dots \}. \quad (2)$$

In expanding the  $n$ th power of  $\mathcal{H}_0$ , each term corresponds to a selection of  $n$  directed nearest-neighbor pairs of lattice sites (some of which may be repeated) which we may represent diagrammatically by a set of  $n$  arrows. The set of  $b(\leq n)$  undirected bonds so covered constitutes a subgraph of the lattice, the shadow graph  $g$ . From the well-known commutation relations satisfied by the operators  $a$  and  $a^\dagger$ , the trace in the subspace of the  $i$ th site will vanish unless (i) there are an equal number of operators  $a_i$  and  $a_i^\dagger$  (equal number of arrow heads and tails), and (ii) there is a regular alternation in the order of  $a_i$  and  $a_i^\dagger$  operators (heads and tails alternate). If (i) and (ii) are satisfied, the trace is unity un-

less no operators are included for the  $i$ th site in which case the trace equals two. To determine  $Z$  we need two kinds of information: (i) a set of weak lattice constants of the shadow graphs, available from work on the Ising and Heisenberg models,<sup>9-11</sup> and (ii) the number of allowable configurations of arrows for each shadow graph. The latter data, peculiar to this problem, have been obtained with the aid of a simple computer program. In this way we have obtained the first nine terms in the partition function for arbitrary lattice. From the zero-field partition function may be obtained the entropy, internal energy, and specific heat. For the fcc lattice the specific-heat series is

$$C/k = 3K^2 + 12K^3 + 32.25K^4 + 90K^5 + 320.8749 \dots K^6 + 1312.1506 \dots K^7 + 5465.5888 \dots K^8 + 22\,505.5368 \dots K^9 + \dots \quad (3)$$

For the Ising and Heisenberg models it is customary also to evaluate the high-temperature parallel susceptibility series, which for zero magnetic field is directly proportional to the square of the fluctuation in the long-range order (parallel magnetization). For the XY model the long-range-order (perpendicular-magnetization) operator,

$$M_\perp = m \sum_i \sigma_{ix}, \quad (4)$$

does not commute with the Hamiltonian, and hence the corresponding (perpendicular) susceptibility is no longer proportional to the square of the fluctuation in the long-range order. For the XY model it is simpler to calculate the latter quantity, namely

$$Y = \sum_{i,j=1}^N \langle a_i^\dagger a_j + a_j^\dagger a_i \rangle$$

$$= -\lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \lambda} \ln \text{tr} \exp\{-\beta[\mathcal{H}_0 + \lambda \sum_{i,j} (a_i^\dagger a_j + a_j^\dagger a_i)]\} / \beta. \quad (5)$$

The calculations for the fluctuation differ from those for the partition function in that one of the arrows is of arbitrary length and occurs always in a fixed position (e.g., first). We have calculated for arbitrary lattice the first seven terms of the square of the fluctuation in the long-range order. For the fcc lattice, the result becomes

$$Y = 1 + 3K + 16.5K^2 + 82K^3 + 397.7917 \dots K^4 + 1918.9375K^5 + 9281.6583 \dots K^6 + 44\,902.3225 \dots K^7 + \dots \quad (6)$$

As with the Ising and Heisenberg models, the critical temperature for the XY model is most precisely estimated from analysis of the series for the fluctuation in the long-range order. Figure 1 shows a conventional ratio plot<sup>12</sup> of the coefficients in the high-temperature expansion of  $Y$  for the fcc lattice from which we estimate  $kT_c/J \equiv K_c^{-1} = 4.84 \pm 0.06$ , and  $\gamma = 1.00 \pm 0.07$  in the asymptotic form

$$Y \approx \Gamma(T - T_c)^{-\gamma}. \quad (7)$$

Padé-approximant<sup>13</sup> analysis yields  $K_c^{-1} = 4.84 \pm 0.05$  and  $\gamma = 1.00 \pm 0.06$ , consistent with the ratio method.

Figure 1 also contains a ratio plot of the coefficients in the high-temperature specific-heat series for the XY model on the fcc lattice. Taking  $K_c^{-1} = 4.84 \pm 0.06$  from the fluctuation-series analysis, we estimate  $\alpha = -0.20 \pm 0.20$ . This value of  $\alpha$  almost certainly indicates that the specific heat of the XY model has at  $T_c$  a finite cusp

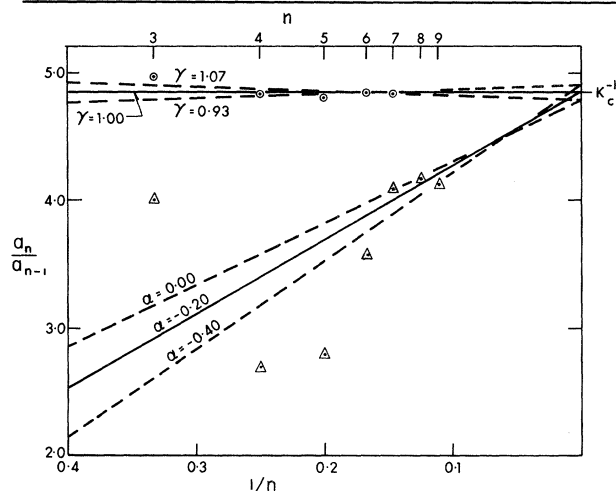


FIG. 1. Ratio of coefficients of the high-temperature series expansion of the square of the fluctuation in the long-range order (open circles) and the specific heat (triangles), both for the XY model on the fcc lattice. Solid lines indicate best fit and dashed lines limits of confidence.

with vertical slope. Baker et al.<sup>14</sup> come to the same conclusions about the Heisenberg model on the basis of somewhat shakier evidence.

Table I summarizes the above data for the XY model and, for comparison, the corresponding data for the Ising and Heisenberg models. We might have expected, because of the "two-dimensional" nature of the interaction in the XY model as opposed to "one-dimensional" and "three-dimensional" interaction in the Ising and Heisenberg models, respectively, that the critical values for the XY model would represent some interpolation between those for the Ising and Heisenberg models. In fact, the situation is more complicated. The singularity in the square of the fluctuation in the long-range order for the XY model is less sharp than even in the Ising model. The cusp in the specific heat resembles closely that for the Heisenberg model. The crit-

ical temperature is nearly the same as that for the Ising model.

Presumably, the perpendicular susceptibility series would have a singularity very similar to that of the square of the fluctuation, but the series is much more tedious to evaluate and we do not yet have many terms. We have also obtained the first six terms in the high-temperature expansion of the parallel susceptibility, which agree exactly with the results of Obokata, Ono, and Oguchi<sup>7</sup> and Pirnie.<sup>8</sup> Because the parallel susceptibility,  $\partial M_z/\partial H_z$ , of the XY model is expected to resemble the perpendicular susceptibility of the Ising model, little can be expected of the series. This expectation is in accord with the results; the first six terms of the parallel susceptibility series are very irregular.

Finally, we may consider comparison with experiment. For  $\text{Gd}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$ , Wielinga, Lubbers, and Huiskamp<sup>3</sup> have estimated for the low-temperature side of  $T_C$  the specific-heat critical index  $\alpha' = 0.60$ . For  $T > T_C$  the data are much too scattered to make a reliable estimate of  $\alpha$ . Also, because of the importance of dipolar coupling term, the XY model has limited relevance for this substance.

As mentioned above,<sup>2</sup> the XY model was first introduced as a model of a hard-core Bose fluid, so the theoretical results may be compared with the results of experiment<sup>15</sup> on liquid He<sup>4</sup>. A cusp of vertical slope may be difficult to distinguish experimentally from an infinity in the specific heat. However, the probable cusp height of approximately  $R/2$  in the XY model seems in definite conflict with experiment. Presumably the attractive tail of the intermolecular potential in helium cannot be neglected if one is to obtain, *inter alia*, an infinite specific heat.

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Table I. Critical data for the XY model compared with previous work on the Heisenberg model and the Ising model, all for the fcc lattice.

Model	$kT_c/J$	$\gamma$	$\alpha$	Height of Singularity, $C(T_c)/k$	Critical Entropy, $S_c/k$
XY	$4.84 \pm 0.06$	$1.00 \pm 0.07$	$-0.20 \pm 0.20$	$0.49_{0.01}^{+\infty}$	$0.557 \pm 0.001$
Heisenberg <sup>a</sup>	4.013	1.43	$-0.20 \pm 0.05$	$1.0 \pm 0.2$	0.355
Ising <sup>b</sup>	4.897	5/4	$\frac{1}{8}$	$\infty$	0.591

<sup>a</sup>See Ref. 14.

<sup>b</sup>See Ref. 1 and D. L. Hunter, thesis, University of London King's College, 1967 (unpublished).

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<sup>1</sup>M. E. Fisher, Rept. Progr. Phys. 30, 615, (1967).

<sup>2</sup>T. Matsubara and H. Matsuda, Progr. Theoret. Phys. (Kyoto) 16, 416 (1956).

<sup>3</sup>R. F. Wielinga, J. Lubbers, and W. J. Huiskamp, Physica 37, 375 (1967). We are grateful to Professor Huiskamp for sending us a copy of their results prior to publication.

<sup>4</sup>Ref. 1, Sec. 4.3.

<sup>5</sup>R. Whitlock and P. R. Zilsel, Phys. Rev. 13, 2409 (1963).

<sup>6</sup>C. N. Yang and C. P. Yang, Phys. Rev. Letters 13, 303 (1964), and Phys. Rev. 147, 303 (1966).

<sup>7</sup>T. Obokata, I. Ono, and T. Oguchi, J. Phys. Soc. Japan 23, 516 (1967).

<sup>8</sup>K. Pirnie, unpublished. We are grateful to Dr. Pirnie for informing us of his results prior to publica-

tion.

<sup>9</sup>C. Domb, Advan. Phys. 9, 149 (1960).

<sup>10</sup>M. F. Sykes, J. W. Essam, B. R. Heap, and B. J. Hiley, J. Math. Phys. 7, 1557 (1966).

<sup>11</sup>G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Brookhaven National Laboratory Report No. BNL-50053 (T-460), 1967 (unpublished).

<sup>12</sup>C. Domb and M. F. Sykes, Proc. Roy. Soc. (London), Ser. A 240, 214 (1957); Ref. 1, Sec. 7.2.

<sup>13</sup>G. A. Baker, Phys. Rev. 122, 1477 (1961), and in Advances in Theoretical Physics, edited by K. A. Brueckner (Academic Press, Inc., New York, 1965), Vol. I, p. 1.

<sup>14</sup>G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Rev. 164, 800 (1967).

<sup>15</sup>W. M. Fairbank and C. F. Kellers, in Critical Phenomena, Proceedings of a Conference, Washington, D. C., 1965, edited by M. S. Green and J. V. Sengers, National Bureau of Standards Miscellaneous Publication No. 273 (U.S. Government Printing Office, Washington, D. C., 1966), p. 71.

## EXPRESSIONS FOR THE TRANSMISSION COEFFICIENTS AND THE MEAN SQUARE DEVIATION OF THE ELASTIC-SCATTERING CROSS SECTION

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An expression for the transmission coefficient for the general case of an arbitrary number of open channels, valid for all values of the ratio of the average partial width to the average spacing, is obtained from a completely unitary matrix. For the purely elastic-scattering case, the average value and the mean-square deviation of the elastic-scattering cross section are expressed in terms of the potential-scattering phase shift and the ratio of the average width to the average spacing.

In the statistical study of the low-energy nuclear reactions which pass through the formation of a compound nucleus, one tries to express the average quantities like the transmission coefficients<sup>1</sup> and the average cross sections<sup>2</sup> in terms of the averages of the resonance parameters of the low-energy collision matrix. The resonance parameters which enter into the expressions for the average quantities are the partial widths and the spacings of the poles of the collision matrix. The two main difficulties in deriving these results have been (1) keeping track of the unitary condition on the resonance-pole expansion form of the low-energy collision matrix, and (2) validity of the expressions for all values of the ratio of the average partial width to the average spacing. Our aim in this note is to show that exact expressions for the transmission coefficients and the average cross sections can be obtained if we start from the pole-resonance form of the unitary matrix, which has been given recently by

us.<sup>3</sup>

We have recently shown<sup>3</sup> that the unitary pole-resonance form of the collision matrix  $U$ , based on  $R$ -matrix theory<sup>4</sup> or Feshbach's unified theory of nuclear reactions,<sup>5</sup> can always be written as

$$U(E) = V \left[ 1 - i \sum_{\mu=1}^N \frac{G_{\mu}}{E - z_{\mu}} \right] V, \quad (1)$$

where  $z_{\mu} = \mathcal{E}_{\mu} - \frac{1}{2}i\Gamma_{\mu}$  are the complex poles, and the matrix elements of  $G_{\mu}$  are the complex width amplitudes. The matrix  $V$  gives rise to direct reactions and for the case of  $m$  channels can be written as

$$V = O d \tilde{O}, \quad (2)$$

where  $O$  is an  $m \times m$  real orthogonal matrix and  $d$  is a diagonal matrix, the elements of which are  $d_{cc'} = \exp(-i\varphi_c) \delta_{cc'}$ .

We first consider the purely elastic-scattering