

¹³Except only as regards $g_{3,8}$, for each lattice, where discrepancies of the order of 1 in 10^9 reflect round-off error in the $F_4^*(8)$ entries of I, as noted therein.

¹⁴See E. T. Copson, *Functions of a Complex Variable* (Oxford U.P., Oxford, 1935), p. 125.

¹⁵For present purposes, PA's are adequately defined in I. We continue to use the notation $[D, N]$ to denote the PA which has as numerator a polynomial of degree N and as denominator a polynomial of degree D . $D+N$ equals the number of terms in the given series which are used in constructing the approximant. For series whose coefficients are known through x^8 , we shall hope to find reasonable convergence between conclusions drawn from the $[3, 3]$, $[3, 4]$, $[4, 3]$, $[4, 4]$, $[3, 5]$, and $[5, 3]$ approximants.

¹⁶F. J. Dyson, Phys. Rev. **102**, 1230 (1956).

¹⁷The extra terms, up to $(T/T_c)^4$, given by Dyson increase $1-M$ by about 7% when $T/T_c=0.3$ and by about 14% when $T/T_c=0.5$.

¹⁸J. F. Cooke and H. A. Gersch, Phys. Rev. **153**, 641 (1967).

¹⁹See Ref. 18, and Ref. 3, p. 102.

²⁰N. D. Mermin and H. Wagner, Phys. Rev. Letters **17**, 1133 (1966).

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²²L. J. de Jongh, A. C. Botterman, F. R. de Boer, and A. R. Miedema, J. Appl. Phys. **40**, 1363 (1969).

²³J. W. Essam and M. E. Fisher, J. Chem. Phys. **38**, 802 (1963).

²⁴This result is not confined to first-order spin-wave theory. The best references, for which we are indebted to Professor M. E. Fisher, are V. G. Vaks, A. I. Larkin, and S. A. Pikin, Zh. Eksperim. i Teor. Fiz. **53**, 281 (1968); **53**, 1089 (1968) [Soviet Phys. JETP **26**, 188 (1968); **26**, 647 (1968)].

²⁵We recall that in I, from somewhat longer series examined in a variety of ways, γ was found to be close to 1.43 for the Heisenberg spin- $\frac{1}{2}$ problem.

²⁶D. S. Gaunt and G. A. Baker, Jr., Phys. Rev. B **1**, 1184 (1970), Table III.

²⁷It is convenient to work in terms of $(T_c - T)/T_c$ rather than $T_c - T$ although, of course, this in no way affects the conclusions. And where no confusion can arise, we shall drop the suffix zero from M_0 .

²⁸Nonclassical exponents are normally derived as the residues of PA's at poles. For the Ising model $M_0(T)$ is known explicitly as a power series in $\exp(-2J/\kappa T)$, and $\partial \ln M_0 / \partial T$ can be examined in the neighborhood of T_c . See G. A. Baker, Jr., Phys. Rev. **124**, 768 (1961) or Ref. 23.

²⁹This is true also of the Ising model, but not of the "classical" ($s=\infty$) Heisenberg model. See R. E. Watson, M. Blume, and G. H. Vineyard, Phys. Rev. **181**, 811 (1969).

³⁰The increased gradient in the region near $M=0.2$ is simply due to irregularity in the approximants, and has nothing to do with the ultimate limit of 0.5 discussed above.

³¹In drawing up Table VII we have, for each approximation, used for x_c the value given by the corresponding entry in the bottom line of Table II. Had we instead used always $x_c=0.2492$ there would have been some changes in the numbers in Table VII, but our conclusion would have been unaltered.

³²D. S. Gaunt, M. E. Fisher, M. F. Sykes, and J. W. Essam, Phys. Rev. Letters **13**, 713 (1964); D. S. Gaunt, Proc. Phys. Soc. (London) **92**, 150 (1967).

³³A further argument, leading to the same conclusions, is given in Gaunt and Baker, Ref. 26.

³⁴It might be thought that some of these uncertainties would be avoided if we were to start from Eq. (22) and derive directly a series expansion for δ^* of the form $\Sigma_{n \geq 0} c_n(t) x^n$ where the coefficients $c_n(t)$ are finite polynomials which are known exactly. Unfortunately, PA's to this series, evaluated at x_c for fixed t , fail to converge at all over the interesting range of t .

³⁵The same result, but with weaker limits, comes from analysis of the series for the bcc and sc lattices.

³⁶R. F. Wielinga, thesis, Leiden, 1968, Chap. V, Fig. 6 (unpublished).

Susceptibility and Fluctuation. II.

Determination of the Frequency Moments*

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The frequency moment appearing in a relation between susceptibility and fluctuation is expressed in terms of measurable quantities. A discussion is given of a determination of the critical exponent for the staggered magnetic susceptibility of RbMnF_3 .

I. INTRODUCTION

In a discussion¹ of the relation between the critical exponents of susceptibility and of fluctuation

near a critical temperature T_c a frequency moment of a spectral density was introduced. If this moment $\bar{\omega}$ goes to zero at T_c , these two critical exponents are equal. In the present work $\bar{\omega}$ is re-

lated to the high-frequency behavior of a generalized frequency-dependent susceptibility. This in turn is measurable via inelastic neutron scattering from magnetic materials.² These results make precise the relation of $\bar{\omega}$ to moments calculated for magnetic models and to the phenomenon of slowing down of fluctuations observed near T_c . The results are applied to RbMnF₃: The staggered magnetic susceptibility and fluctuations of the staggered magnetization are equal to within $\frac{1}{2}\%$ at temperatures above T_N .

II. DETERMINATION OF THE FREQUENCY MOMENT

Following the notation of I, the susceptibility χ_T and fluctuation $S^{(0)}$ for the spatial Fourier transform A_k of a magnetization operator are

$$\chi_T = \int_0^\beta d\lambda \langle \Delta A_k(\lambda) \Delta A_k^\dagger \rangle_0, \quad (1)$$

$$S^{(0)} = \frac{1}{2} \langle \{ \Delta A_k, \Delta A_k^\dagger \} \rangle_0. \quad (2)$$

These are related by the following inequalities:

$$(\tanh y_k)/y_k \leq \chi_T/(\beta S^{(0)}) \leq 1, \quad (3)$$

in which y_k is the root of

$$y_k \tanh y_k = \frac{1}{2} \beta \bar{\omega}_k, \quad (4)$$

and $\bar{\omega}_k$ is defined by

$$\bar{\omega}_k = \langle [A_k, [H_0, A_k^\dagger]] \rangle_0 / (2S^{(0)}). \quad (5)$$

The numerator in $\bar{\omega}_k$ appears also in the study of a frequency-dependent susceptibility. In the theory of linear response² this is defined to be

$$\chi_{A_k A_k^\dagger}(\omega) = \lim_{\epsilon \rightarrow 0^+} (-i) \int_0^\infty dt e^{-i\omega t - \epsilon t} \langle [A_k, e^{iH_0 t} A_k^\dagger e^{-iH_0 t}] \rangle_0.$$

Define a symmetrized susceptibility: (6)

$$\chi(k, \omega) = \frac{1}{2} [\chi_{A_k A_k^\dagger}(\omega) + \chi_{A_k^\dagger A_k}(\omega)]. \quad (7)$$

At high frequencies the real part of this susceptibility is proportional to the numerator of Eq. (5):

$$\text{Re } \chi(k, \omega) \cong -\langle [A_k, [H_0, A_k^\dagger]] \rangle_0 / \omega^2 + O(1/\omega^4). \quad (8)$$

The real and imaginary parts of the susceptibility are related by a Kramers-Kronig relation (P denotes the principal-value integral):

$$\text{Re } \chi(k, \omega) = \frac{P}{\pi} \int_{-\infty}^{\infty} d\omega' \omega' \text{Im } [\chi(k, \omega')] / (\omega^2 - \omega'^2). \quad (9)$$

The imaginary part of the susceptibility determines the partial differential cross section for momentum transfer k and energy transfer ω in the inelastic scattering of neutrons³:

$$\frac{d^2\sigma}{d\Omega d\omega} \propto (1 - e^{-\beta\omega})^{-1} \text{Im } \chi(k, \omega). \quad (10)$$

Because the absolute scale of $\text{Im } \chi$ may not be

known in such measurements, a dimensionless quantity $\bar{\Omega}$ is defined:

$$\bar{\Omega} = \beta^2 \int_{-\infty}^{\infty} d\omega \omega \text{Im } [\chi(k, \omega)] / \{ P \int_{-\infty}^{\infty} d\omega \text{Im } [\chi(k, \omega)] / \omega \}. \quad (11)$$

The relation of this to the energy in Eq. (4) is⁴

$$\beta \bar{\omega}_k = \bar{\Omega} \chi_T / 2\beta S^{(0)} \quad (12)$$

$\bar{\omega}_k$ is also related to the second moment of a spectral shape function defined by other workers² as $F^{(2)}$:

$$F^{(2)} = \langle [A_k, [H_0, A_k^\dagger]] \rangle_0 / \chi_T = \bar{\Omega} / \beta^2. \quad (13)$$

This moment has been evaluated for theoretical models in various temperature ranges; one such result is used in Sec. III.

In the phenomenon of critical slowing down,² for momentum transfers close to reciprocal magnetic lattice points k_0 the energy width of the partial differential cross section narrows drastically as the critical temperature is approached. This is a property of $\text{Im } \chi(k, \omega)$ and reduces the frequency moment $\bar{\omega}$ through Eq. (11) and Eq. (12). While a Lorentzian energy shape fitted to the experiments⁵ does not yield a convergent numerator in Eq. (11), a plausible cutoff of the Lorentzian permits an order-of-magnitude determination of $\bar{\Omega}$ from inelastic neutron scattering experiments. Such a calculation is described in Sec. III.

III. APPLICATION TO RbMnF₃

Inelastic neutron scattering measurements on RbMnF₃ near T_N have been analyzed⁶ to yield the critical exponent of the staggered magnetic susceptibility. The quantity directly determined in the experiment is the critical exponent of the fluctuation of the staggered magnetization. RbMnF₃ is a cubic Heisenberg antiferromagnet with essentially nearest-neighbor interactions⁷; therefore an argument already given¹ in I establishes the equality of these two critical exponents. The calculations here show that the difference between the susceptibility and fluctuation is small even at temperatures far from T_N .

For room temperature ($T \approx 3.5 T_N$) the measured nearest-neighbor coupling can be used in a high-temperature expansion for the second moment.⁸ Eq. (13), to calculate $\bar{\Omega}$ for k equal to the first antiferromagnetic reciprocal-lattice point k_0 . The result is $\bar{\Omega} = 2.7 \times 10^{-2}$. Application of a set of inequalities obtained from Eqs. (3), (4), and (12) yields

$$(1 + \frac{1}{12} \bar{\Omega})^{-1} \leq \chi_T / (\beta S^{(0)}) \leq 1, \quad (14)$$

which then establishes the equality of χ_T and $\beta S^{(0)}$ to within 0.3%.

For temperatures near T_N the measured shape⁵

of the inelastic scattering for momentum transfer equal to k_0 can be used. An analysis of such measurements in terms of a Lorentzian shape with energy half-width Γ has been reported⁵ for $T > T_N$. As remarked in Sec. II, this approximation to the line shape does not yield a convergent integral for $\bar{\Omega}$ in Eq. (11). If the measurement at $T - T_N = 8$ K is used with a Lorentzian cutoff at energy transfer 5Γ , the result is $\bar{\Omega} = 7.2 \times 10^{-3}$. If the cutoff is at 10Γ , the result is $\bar{\Omega} = 1.6 \times 10^{-2}$. Even with the larger cutoff, the maximum possible difference here between χ_T and $\beta S^{(0)}$ is only 0.14%. The ex-

perimental width Γ decreases on further approach to T_N , and the possible deviation between χ_T and $\beta S^{(0)}$ also decreases.

A more precise application of such measurements to this topic and to the determination of the second moment $F^{(2)}$ will depend on improved measurements of the spectral shape function at large energy transfers.

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²W. Marshall and R. D. Lowde, Rept. Progr. Phys. **31**, 705 (1968).

³For conditions on the validity of this expression see Ref. 2.

⁴This omits the distinction between the static susceptibility calculated from linear response theory and the isothermal susceptibility [H. Falk, Phys. Rev. **165**, 602 (1968)]. If the distinction is maintained the $\bar{\omega}$ calculated from Eqs. (11) and (12) is an upper bound to the

$\bar{\omega}$ in Eq. (5). Use of it in Eqs. (3) and (4) still yields a lower bound for $\chi_T/\beta S^{(0)}$. These remarks do not apply to Eqs. (12) and (13) used together.

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General Lattice Model of Phase Transitions

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A general lattice-statistical model which includes all soluble two-dimensional model of phase transitions is proposed. Besides the well-known Ising and "ice" models, other soluble cases are also considered. After discussing some general symmetry properties of this model, we consider in detail a particular class of the soluble cases, the "free-fermion" model. The explicit expressions for all thermodynamic functions with the inclusion of an external electric field are obtained. It is shown that both the specific heat and the polarizability of the free-fermion model exhibit in general a logarithmic singularity. An inverse-square-root singularity results, however, if the free-fermion model also satisfies the ice condition. The results are illustrated with a specific example.

I. INTRODUCTION

Considerations of the phenomena of phase transitions have been, to a large extent, centered around the study of lattice systems. Besides the intrinsic interest surrounding the lattice systems

as models of real physical situations, one is further attracted to their consideration by the possibility of obtaining exact nontrivial solutions. But the soluble problems are very few in number. The Ising model^{1,2} of magnetism, first proposed some