

In conclusion, the angular distribution of the magnetic scattering in chromium can be described, as in other $3d$ metals, in terms of $3d$ free-atom form factors. The data are best fitted by having a 60%- $3d$ -orbital-40%- $3d$ -spin contribution to the induced moment both above and below the anti-ferromagnetic transition temperature. The orbital and spin susceptibilities, for our samples, were found to be $(98 \pm 3) \times 10^{-6}$ emu/mole and $(65 \pm 2) \times 10^{-6}$ emu/mole, respectively. These results are consistent with measurements of the total susceptibility and gyromagnetic ratio of chromium. The magnitude of the localized induced moment has been found to be essentially temperature independent, in the 25–100°C temperature region. Thus we do not observe the characteristic temperature dependence expected from an intrinsic localized spin.

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Neutron Scattering and the Correlation Functions of the Ising Model near T_c

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We study near T_c the correlation function $\langle \sigma_{00} \sigma_{MN} \rangle$ of the two-dimensional Ising model.

In this Letter we present the results of our computation of the Fourier transform of the spin-spin correlation function $\langle \sigma_{00} \sigma_{MN} \rangle$ for the two-dimensional Ising model in the scaling limit $T \rightarrow T_c$, $R = (N^2 + M^2)^{1/2} \rightarrow \infty$ with $(T - T_c)R$ fixed and of order 1.¹ We use these results to show that the asymptotic formula of Fisher and Langer² provides a much better method of extracting the critical exponent η from neutron scattering data than do the formulas of Fisher³ and Fisher and Burford.⁴

More specifically, we have computed

$$F_{\pm}(t) = \lim R^{1/4} \langle \sigma_{00} \sigma_{MN} \rangle \quad (1)$$

in the scaling limit, where $t = \kappa R$, κ is the inverse

correlation length $[\sim 2 \ln(1 + \sqrt{2}) |T/T_c - 1|$ for the isotropic Ising model], and the subscripts $+$, $-$ refer to above and below T_c , respectively. The momentum-dependent susceptibility is

$$\chi(\vec{k}, T) = \sum_{M=-\infty}^{\infty} \sum_{N=-\infty}^{\infty} e^{i\vec{k} \cdot \vec{R}} (\langle \sigma_{00} \sigma_{MN} \rangle - \mathfrak{R}^2), \quad (2)$$

where \mathfrak{R}^2 is the long-range order parameter. In the scaling region we define

$$X_{\pm}(y) = \lim_{\kappa \rightarrow 0} \kappa^{\gamma/\nu} \chi(\vec{k}, T), \quad (3)$$

where $y = k/\kappa$ is fixed and of order 1.

We have evaluated $X_{\pm}(y)$ and these are plotted in Fig. 1 for y not too large. For large y (> 20) the asymptotic expansions given below, in Eq.

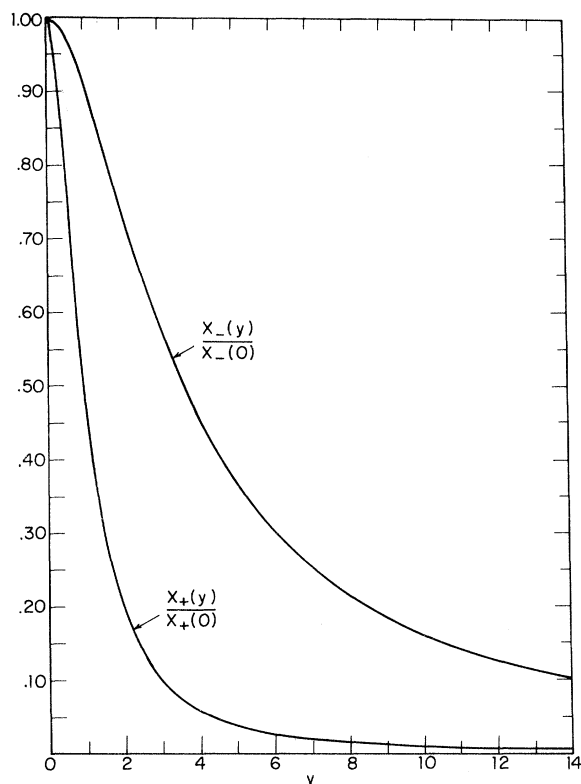


FIG. 1. The scale functions $X_{\pm}(y)/X_{\pm}(0)$, where $X_{\pm}(0)$ are given by (19).

(15), are accurate to five significant figures.

Assuming that inelasticity effects are negligible⁵ and that multiple scattering may be neglected, then the neutron cross section is proportional to $\chi(\vec{k}, T)$. The critical exponent η is then de-

fined from $X_{\pm}(y)$ by the limiting behavior

$$x_{\pm}(y) \rightarrow x_1 y^{-2+\eta} \text{ as } y \rightarrow \infty. \quad (4)$$

Unfortunately, it is not possible to perform the mathematical limit of (4) in the laboratory (there exist virtually no data in the scaling region for $y > 50$, and $y \approx 30$ is perhaps typical⁶). Therefore, in order to make contact with this definition it is necessary to extrapolate the data using some phenomenological formula. The most popular form used to fit the data is that of Fisher,³

$$X_F(y) = A(1 + y^2)^{\eta/2-1}. \quad (5)$$

An improved form is that of Fisher and Burford,⁴

$$X_{FB}(y) = A(1 + By^2)^{\eta/2}(1 + y^2)^{-1}. \quad (6)$$

Both (5) and (6) have been proposed for $T > T_c$, and reduce to (4) as $y \rightarrow \infty$.

We have used our computed values of $X_{\pm}(y)$ as data and performed a least-squares fit using $X_F(y)$ and $X_{FB}(y)$ (see Table I). If we use a range of y which includes $y=0$ and cut off at some limit of the order 30 to 50, we find that $X_{FB}(y)$ gives $\eta \approx 0.10$, while $X_F(y)$ with a range of $0 \leq y \leq 10$ gives $\eta \approx 0.02$. This situation is improved by not using the data around $y=0$. For example, for 100 points over the range $20 \leq y \leq 60$, $X_F(y)$ gives $\eta \approx 0.13$ and $X_{FB}(y)$ gives $\eta \approx 0.18$. $X_{FB}(y)$ fits the data quite well in the sense that the computed values from the fitted $X_{FB}(y)$ reproduce the input values of $X_{\pm}(y)$ to three to four significant figures. Yet, there is an error of approximately 30% in the predicted η , and nearly 50% error in the predicted η from $X_F(y)$.

TABLE I. This table gives the predicted critical exponent η from a least-squares fit to a phenomenological formula. The formulas are given in the left-hand column. The upper row gives the interval over which the formula was fitted. The number of data points, which are equally spaced and equally weighted, is also given. The upper (lower) value of η is for data above (below) T_c . The asterisk means that some of the fitted values differ from the input values by 1% or more.

| | (10, 30) 50 points | (20, 40) 50 points | (20, 60) 100 points | (20, 140) 300 points | (20, 200) 450 points |
|---------------------------------------|-----------------------|-----------------------|------------------------|-------------------------|-------------------------|
| $X_F(y)$ | 0.086* | 0.123 0.441* | 0.131* 0.421* | 0.142* 0.397* | 0.144* 0.392* |
| $X_{FB}(y)$ | 0.143 | 0.168 | 0.176 | 0.188 | 0.191* |
| $Ay^{\eta-2}$ | 0.095 | 0.125 0.443* | 0.133* 0.423* | 0.143* 0.399* | 0.145* 0.393* |
| $Ay^{\eta-2}$ $+By^{\eta-3} \ln y$ | 0.299* | 0.264 0.241 | 0.260 0.243 | 0.256 0.245 | 0.256 0.245 |

The reason for these large errors is that $X_F(y)$ and $X_{FB}(y)$ are not really valid in the range of experimentally accessible y . The “ η ” appearing in these formulas is the true η only when (4) is a good approximation. When (4) is not a good approximation, we must consider higher-order terms in $X_{\pm}(y)$, i.e., [see (15)]

$$X_{\pm}(y) \sim x_1 y^{-2+\eta} [1 \pm (x_2 y^{\alpha/\nu} + x_3) y^{-1/\nu}]. \quad (7)$$

(For the two-dimensional Ising model $\alpha=0$ and $\nu=1$ and $y^{\alpha/\nu}$ is replaced by $\ln y$.) Form (7) has been discussed by Fisher and Langer.² With the same data, form (7) with $y^{\alpha/\nu} \rightarrow \ln y$ and $x_3=0$ predicts from a least-squares fit an η with only 4% error. If we use (7) with $\nu=1$ and, say, $x_3=x_2$, then the fitting program gives an equally good η and $\alpha/\nu = -0.078$.

We should point out that (1) η in the two-dimen-

sional Ising model is a large effect since three-dimensional η 's range from one fourth to one fifth as large^{4,7}; (2) the value $\alpha=0$ makes the second-order term a minimal effect in two dimensions, there being evidence that $\alpha \neq 0$ in three dimensions.⁸ Thus, if a phenomenological formula is unable to extract η from our “data,” then we feel this is a strong reason, especially in light of points (1) and (2), to reject this phenomenological formula. Therefore, we conclude that (7) provides a much better method of extracting η than do (5) and (6).

We commence our study of $F_{\pm}(t)$ by evaluating the expansion for $\langle \sigma_{00} \sigma_{MN} \rangle$ derived by Cheng and Wu⁹ to all orders. Letting $T \rightarrow T_c$ and $R \rightarrow \infty$, we verify that if the horizontal and vertical interaction energies E_1 and E_2 are equal, then $\langle \sigma_{00} \times \sigma_{MN} \rangle R^{1/4}$ becomes cylindrically symmetric. More importantly, we see that if $X_{\pm}(y)$ is represented as a dispersion integral,

$$X_{\pm}(y) = \int_0^{\infty} dy' \frac{\rho_{\pm}(y')}{y^2 + y'^2} = \sum_{n=1}^{\infty} \int_0^{\infty} dy' \frac{\rho_{\pm}^{(n)}(y')}{y^2 + y'^2} \equiv \sum_{n=1}^{\infty} X^{(n)}(y), \quad (8)$$

where $\rho_{\pm}^{(1)}(y)$ is a multiple of $\delta(y-1)$ and for $n \geq 2$ $\rho_{\pm}^{(n)}(y')$ is zero for $y' < n$ and has no singularities for $n < y'$, then $\rho_{+}^{(2n)}(y') = 0$ and $\rho_{-}^{(2n+1)}(y') = 0$.

We find, upon scaling the leading terms given in Cheng and Wu,

$$X_{+}^{(1)}(y) = 2^{11/8} (1+y^2)^{-1}, \quad (9a)$$

$$X_{-}^{(2)}(y) = 2^{11/8} \pi^{-1} \left[\frac{3}{4} F(3, 1; \frac{3}{2}; -\frac{1}{4}y^2) - \frac{2}{3} (1 + \frac{1}{4}y^2) F(3, 2; \frac{5}{2}; -\frac{1}{4}y^2) + \frac{9}{15} (\frac{1}{4}y^2) (1 + \frac{1}{16}y^2) F(3, 3; \frac{7}{2}; -\frac{1}{4}y^2) \right], \quad (9b)$$

where $F(a, b; c; z)$ is the hypergeometric function. It is clear from (9a) that $X_{+}^{(1)}(y)$ is the Ornstein-Zernike pole. However, in $X_{-}^{(2)}(y)$ the singularity at $y = \pm 2i$ is not a pole but a cut.

We can also use the expansion of Cheng and Wu to study the approach to the scaling limit. For $T > T_c$ the first term of the expansion gives as an approximation for the susceptibility $\chi(\vec{k}, T)$

$$\chi^{(1)}(k_x, k_y, T) = [(\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2} - 1]^{1/4} (\gamma_1 \gamma_2)^{1/2} \Delta^{-1}(k_x, k_y); \quad (10)$$

$\Delta(k_x, k_y) = a - \gamma_1 \cos k_x - \gamma_2 \cos k_y$, $a = (1 + z_1^2)(1 + z_2^2)$, $\gamma_1 = 2z_2(1 - z_1^2)$, $\gamma_2 = 2z_1(1 - z_2^2)$, $z_i = \tanh(\beta E_i)$, and $\beta^{-1} = k_B T$. For $T < T_c$ we restrict our attention to $k=0$ and find

$$\chi^{(2)}(0, T) = [1 - (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2}]^{1/4} (24\pi)^{-1} \gamma_1 \gamma_2 \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\varphi_1 d\varphi_2 \cos \varphi_1 \cos \varphi_2 \Delta^{-2}(\varphi_1, \varphi_2). \quad (11)$$

To obtain the expansion for t small we consider the ratio $x_0(N) = \langle \sigma_{00} \sigma_{0N-1} \rangle / \langle \sigma_{00} \sigma_{0N} \rangle$ in the scaling limit and use the work of Wu¹⁰ which shows that it is given by

$$x_0^{\pm}(N) = \max(1, \alpha_2) + \kappa \pi \lim_{Z \rightarrow \infty} [-Z^{1/2} (Z+1)^{1/2} \pi^{-1} + \lim_{s \rightarrow 0} (\pi s)^{1/2} \bar{x}(s; Z) - \pi^{1/2} \lim_{s \rightarrow t} \frac{\bar{x}(s; Z)}{\tilde{x}_{\pm}(s)} \lim_{s \rightarrow 0} s^{1/2} \tilde{x}_{\pm}(s)], \quad (12)$$

where $\tilde{x}_{\pm}(s)$ and $\bar{x}(s; Z)$ are solutions to the integral equations

$$\int_0^t K_0(|s-s'|) \tilde{x}_{\pm}(s') ds' = e^{\mp s} \quad (13a)$$

and

$$\int_0^t K_0(|s-s'|) \bar{x}(s'; Z) ds' = Z^{1/2} e^{-Zs}, \quad (13b)$$

and $\alpha_2 = z_1^{-1}(1+z_2)(1-z_1)^{-1}$.

Equation (13) may be solved iteratively when t is small by Pearson's method.¹¹ We obtain¹²

$$F_{\pm}(t) = F(0) \left[1 \pm \frac{1}{2} t \Omega + \frac{1}{16} t^2 \pm \frac{1}{32} t^3 \Omega + O(t^4 \Omega^2) \right], \quad (14)$$

where $\Omega = \ln(t/8) + \gamma_E$, γ_E is Euler's constant, and $F(0) = 0.645\,002\,44\dots$. From (14) we obtain the large- y expansion of $X_{\pm}(y)$,

$$X_{\pm}(y) = C y^{-7/4} [x_1 \pm (x_2 \ln y + x_3) y^{-1} + x_4 y^{-2} \pm (x_5 \ln y + x_6) y^{-3} + O(y^{-4} \ln^2 y)], \quad (15)$$

where $C = 2^{19/8} \pi$, $x_1 = 0.065\,964\,77\dots$, $x_2 = 0.105\,981\,71\dots$, $x_3 = 0.026\,046\,69\dots$, $x_4 = -0.012\,620\,7\dots$, $x_5 = -0.050\,092\,92\dots$, $x_6 = 0.056\,712\,79\dots$.

To obtain $F_{\pm}(t)$ at intermediate values of t , we make use of the work of Myers¹³ that expresses the solution to (13) in terms of a Painlevé function $\eta(\theta)$ of the third kind¹⁴ where

$$\eta'' = \eta^{-1}(\eta')^2 - \eta^{-1} + \eta^3 - \theta^{-1}\eta'; \quad (16a)$$

$$\eta(\theta) = -\theta(\ln \frac{1}{4}\theta + \gamma_E) + O(\theta^5 \ln^3 \theta) \text{ as } \theta \rightarrow 0; \quad (16b)$$

$$\eta(\theta) = 1 - 2\pi^{-1}K_0(2\theta) + 2\pi^{-2}K_0^2(2\theta) + O(e^{-6\theta}) \text{ as } \theta \rightarrow \infty. \quad (16c)$$

We find

$$F_{\pm}(t) = \frac{1}{2}(2t)^{1/4} [1 \mp \eta(t/2)] \eta^{-1/2}(t/2) \exp \left\{ \int_{t/2}^{\infty} dx (x/4\eta^2) [(1 - \eta^2)^2 - \eta'^2] \right\}. \quad (17)$$

We have numerically solved (16), and by use of (17) numerically interpolated between (14) and the Fourier transform of (9). We have also numerically evaluated $X_{\pm}(y)$ to five significant places. When $y \rightarrow 0$ these evaluations have been carried out to higher accuracy, and we find¹⁵

$$\lim_{T \rightarrow T_c^{\pm}} |1 - T/T_c|^{7/4} \chi(0, T) = C_{\pm}, \quad (18)$$

with

$$C_{+} = 0.962\,581\,732\,1\dots = X_{+}(0) [2 \ln(1 + \sqrt{2})]^{-7/4}, \quad (19a)$$

$$C_{-} = 0.025\,536\,971\,8\dots = X_{-}(0) [2 \ln(1 + \sqrt{2})]^{-7/4}. \quad (19b)$$

These are to be compared with the series results¹⁶ $C_{+} = 0.962\,59 \pm 0.000\,03$ and¹⁷ $C_{-} = 0.026 \pm 0.0006$, and the accurate approximate results¹⁸ from (9) of $C_{+} \approx [2 \ln(1 + \sqrt{2})]^{-7/4} 2^{11/8} = 0.961\,797\dots$ and $C_{-} \approx [2 \ln(1 + \sqrt{2})]^{-7/4} 2^{11/8} (12\pi)^{-1} = 0.025\,512\,4\dots$.

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Exact Results for the Eight-Vertex Model in Three Dimensions*

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A generalized duality argument, similar to the treatment of the two-dimensional Ising model by Kramers and Wannier, is used to locate the transition temperature of the eight-vertex model in three dimensions.

In their original treatment of the two-dimensional Ising problem,¹ before Onsager's exact solution,² Kramers and Wannier introduced the dual transformation relating the partition function at high and low temperatures. Making the reasonable assumption of a unique transition temperature T_c , they were able to locate T_c as the invariant point of the transformation, as well as make qualitative statements about the singularity at T_c .

Subsequently, a generalized dual transformation was used by Sutherland³ to locate the transition temperature of the eight-vertex problem in two dimensions, prior to Baxter's exact solution.⁴ Whereas the Ising problem was self-dual, the duality transformation of the eight-vertex problem related models with different interaction parameters, and thus provided no information on the nature of the singularity.

It is the purpose of this Letter to extend the work of Sutherland to the higher-dimension eight-vertex model.

Consider a four-coordinated lattice in any number of dimensions which is loose packed, i.e., it may be divided into two sublattices A and B , where neighbors of A are B , and vice versa. On the edges place arrows, allowing only an even number to point into each vertex. Let us assume N vertices, and hence $2N$ edges. If one vertex configuration is obtained by reversing the arrows of another, these are called conjugate configurations. Let us assign conjugate configurations the same weight, and thus conjugate pairs have weights a , b , c , and d , as in Fig. 1.

Let $Z(a, b, c, d)$ be the partition function for this problem, the eight-vertex model, which physical-

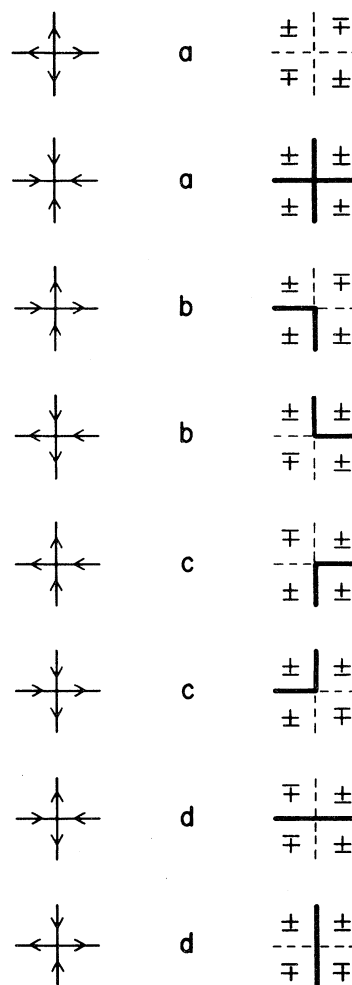


FIG. 1. First column, vertex configurations of arrows for a ferroelectric problem; second column, weights for the eight-vertex model; third column, corresponding bond configurations.