sibility of deducing any meaningful crystal-field parameters from the experimental $g$ value alone. It is possible, however, to obtain these parameters using both the $\Delta E_{T_2-r_g}$ value and the measured $g$ value obtained for the same ion in the same host lattice together. Taking the $\Delta E_{T_2-r_g}$ value and the measured $g$ value for the Pu$^{24+}$ ion in CaF$_2$, the best fit between calculation and experiments can be obtained by using $A_4(r^6) = -600$ cm$^{-1}$ and $A_6(r^8) = 400$ cm$^{-1}$. The $A_4(r^6)$ value is within the $\pm 25\%$ limit of Ref. 1 but the ratio of the sixth- and fourth-order terms, in the notation of $B_6/B_4$, would be $-1.33$ instead of $-0.2$. It should be noted that these parameters can only be considered as a demonstration of the possibility and not as parameters with physical significance at the present time. The reason is that Kolbe and Edelstein deduced the $\Delta E_{T_2-r_g}$ value using matrix elements of the Zeeman and hyperfine interactions calculated with crystal field wave functions which takes into account the crystal field mixing of only two $J$ manifolds. Until these matrix elements are recalculated with the $J$-mixing effect taken fully into account, it is not possible to estimate the error of $\Delta E_{T_2-r_g}$ and the derived crystal field parameters. It should be emphasized that the present discussion has been developed within the framework of the electrostatic model. If the usual assumption of this model, that there is no overlap of the ligand ions with the central ion of interest, is relaxed, then other effects such as orbital reduction, electrostatic-charge penetration, and overt configuration interaction should be taken into account, in addition to the effects discussed, to interpret the experimental results.

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Critical Exponents for the Heisenberg Model

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A recursion relation obtained by Wilson is used for the numerical calculation of critical indices for the $d=3$ classical Heisenberg model. Some of the results obtained are $\gamma = 1.36$ and $\phi = 1.24$.

The renormalization-group (RG) approach to the theory of critical phenomena has been used by Wilson to calculate critical exponents for the $d=3$ Ising model and by Wilson, Fisher, Pfeuty, and Wegner to obtain perturbation expansions in $\epsilon = 4 - d$ of the critical indices for the classical Heisenberg, $X-Y$, and Ising models. Wegner has shown how the RG approach leads to thermodynamic scaling and to deviations from the scaling laws. In this note we report the application of Wilson's recursion relation to the numerical calculation of critical indices for the $d=3$ classical Heisenberg model.

Wilson's formulation, in the $\eta = 0$ approximation, leads to an effective Hamiltonian for spin fluctuations of wave vector $|h| < 2^\ast$, $p$ an integer:

$$
(h_0 T)^{-1} H_p = \int \{ \frac{1}{2} [ \mathbf{\nabla} \mathbf{S}_p(\mathbf{x})]^2 + q_p(\mathbf{S}_p(\mathbf{x})) \} \, d\mathbf{x},
$$

where
where
\[
\mathcal{S}_p(\chi) = 2^{d/2} \int d^d \mathbf{x} d^d \mathbf{y} e^{i(\mathbf{p} \cdot \mathbf{x} - \mathbf{y})} e^{i(\mathbf{p} \cdot \mathbf{y})}.
\] (2)

A continuous distribution of spins is assumed. The effective Hamiltonians for different momentum cutoffs (different \(p\)) are related through the recursion relation\(^\dagger\)
\[
Q_{\mu+1}(\mathbf{z}) = -2^d \ln \left[ \int d^d \mathbf{y} \exp\left[ -y^2 - \frac{1}{2} Q_p(2^{1-d/2} \mathbf{z} + \mathbf{y}) \right] \right]
- \frac{1}{2} Q_p((2^{1-d/2} \mathbf{z} - \mathbf{y})) \right] / \int d^d \mathbf{y} e^{-y^2} Q_p(\mathbf{y}).
\] (3)

At the critical point the length of correlation of spin fluctuations becomes infinite and the series \(\{H_p\} \) or \(\{Q_p\}\) is expected to approach a fixed point \(Q^*(\mathbf{z})\) as \(p \rightarrow \infty\). The critical properties may be determined from the eigenfunctions and eigenvalues of (3) linearized about \(Q^*(\mathbf{z})\).

In order to find \(Q^*(\mathbf{z})\) for the \(d=3\) Heisenberg model we have used the form \(Q_p(\mathbf{z}) = r(\mathbf{z} \cdot \mathbf{z}) + 0.5(\mathbf{z} \cdot \mathbf{z})^2\). Equation (3) was used to compute the series \(\{Q_p(r, z)\}\), integrating numerically by the trapezoidal rule over \(\mathbf{z} / \sqrt{2} + \mathbf{y}\) and \(\mathbf{z} / \sqrt{2} - \mathbf{y}\) with a mesh spacing of \(\Delta = 0.1\) and going out to \(y, z = 4.0\). For \(z > 4.0\), an \(\epsilon^4\) extrapolation was assumed. The parameter \(r\) was varied to find \(r_c\) such that \(Q_p(r_c, z = 1.5) = 0\). The series \(\{r_p\}\) converges to \(r_c\), the critical value, as \(p \rightarrow \infty\). We obtained \(r_c = -3.05232\). This determined the critical point as \(Q_0(r_c, z)\) and an estimate of \(Q^*(z)\) was obtained from the series \(\{Q_p(r_c, z)\}\) for large \(p\).

The linearized recursion relation for deviations about \(Q^*(z)\) is (\(d=3\))
\[
\delta Q_{n+1}(z) = 8 \left\{ \epsilon^{Q^*(z)/\epsilon} \int d^d \mathbf{y} \delta Q_n(\mathbf{z} / \sqrt{2} + \mathbf{y}) \exp\left[ -y^2 - \frac{1}{2} Q^*(\mathbf{z} / \sqrt{2} + \mathbf{y}) - \frac{1}{2} Q^*(\mathbf{z} / \sqrt{2} - \mathbf{y}) \right] - \int d^d \mathbf{y} \delta Q_n(\mathbf{y}) \right\} \times e^{-y^2 \cdot \epsilon Q^*(\mathbf{y})} \int d^d \mathbf{y} e^{-y^2 \cdot \epsilon Q^*(\mathbf{y})}.
\] (4)

The eigenfunctions of the recursion operator may be written as \(\delta Q_{n+1}(z) = f_{n+1}(z)Y^l(\theta, \phi)\), where the \(Y^l(\theta, \phi)\) are spherical harmonics. The quantum number \(l\) is denoted by the symbols \(s, p, d, f, g, \ldots\) for \(l = 0, 1, 2, 3, 4, \ldots\). The function \(f_{n+1}(z)\) obeys
\[
\lambda_{n+1} f_{n+1}(z) = 4 \left\{ \exp\left[ (Q^*(z)/\epsilon - (\epsilon^2/2)) \right] \int d\mu u f_{n+1}(u) \exp\left[ -u^2 - \frac{1}{2} Q^*(u) \right] \right\} d\mu f_{n+1}(u) \exp\left[ -u^2 - Q^*(u) \right] - 2 \int d\mu u f_{n+1}(u) \exp\left[ -u^2 - Q^*(u) \right] / \int d\mu u \exp\left[ -u^2 - Q^*(u) \right],
\] (5)

where \(f_{n+1}(z)\) is a Legendre polynomial.

If one does not normalize \(Q(0) = 0\) as in Eq. (2), which corresponds to a change of the Hamiltonian by a constant, then one obtains \(\lambda_{n+1} = 8\) for the trivial eigenfunction \(\delta Q_n(z) = 0\). An estimate of \(\lambda_{n+1}\) may be obtained from the series \(\{r_p\}\) by noting that \((r_{n+1} - r_n) = \lambda_{n+1} \lambda_{n+1}^2\). A more accurate determination was made by repeated application of the recursion (3) to a trial function with a small (\(\sim 10^{-4}\)) deviation from \(Q^*(z)\). After several iterations, the deviation from \(Q^*(z)\) gives an estimate of \(\delta R_{1+1}(z)\). The value \(\lambda_{n+1} = 2.776\) was obtained, yielding \(y = 2v = 2/10g_2\lambda_{n+1} = 1.357\), in good agreement with the \(\epsilon\) expansions\(^\ddagger\) and also the high-temperature-series calculation of Janssen and Wortis.\(^\ddagger\) At this point it was possible to refine the estimate of \(Q^*(z)\). Repeated applications of (3) could eventually lead to a divergence due to the small contribution of \(\delta Q_{1+1}(z)\) in the original estimate of \(Q^*(z)\). A knowledge of \(\delta Q_{1+1}(z)\) allowed this contribution to be removed, yielding an improved estimate of \(Q^*(z)\), changing by less than one part in \(10^3\) with each iteration.

Deviations from the scaling laws may arise from eigenfunctions of (4) and (5) with eigenvalue \(\lambda \lesssim 1\).

\(\dagger\)See Ref. 5.
\(\ddagger\)See Ref. 6.
A numerical estimate of the largest nontrivial eigenvalue for \( l = 0 \) through \( l = 4 \) was obtained using (5). Repeated applications on a trial function yield the eigenfunction with largest eigenvalue. The integrations were performed by the trapezoidal rule with a mesh spacing of \( \Delta = 0.1 \) and integrating on \( R = (u^2 + 2v^2 - 2\sqrt{2} u v) \) from \( u + \sqrt{2} v \) to \( u + \sqrt{2} v \) and on \( u \) from 0 to 4.0.

For \( l = 0 \) we obtained in this way \( \lambda_4 = 2.783 \), \( \gamma = 1.354 \). A comparison with the previous result \( \lambda_4 = 2.776 \), \( \gamma = 1.357 \) gives an estimate of the error involved in these numerical routines. Using the \( \lambda_2 \) eigenfunction obtained previously, Eq. (7) gives an estimate \( \lambda_2 \approx 0.52 \).

The other results obtained were \( \lambda_{1b} = 5.657 \), \( \lambda_{1d} = 3.547 \), \( \lambda_{2b} = 1.997 \), and \( \lambda_{2d} = 0.9636 \) (see Table I). Notice that \( \log_2 \lambda_{1b} = 2.5 = \frac{2}{3} d + 1 \). This result may also be obtained exactly from (3), and it offers an independent check on our results. From \( \lambda_{od} \) and \( \lambda_{1s} \) one obtains the estimate \( \phi = \nu \log_2 \lambda_{od} = 1.237 \), or, using the estimate \( \nu = 0.7 \) obtained by Jasnow and Wortis, one finds \( \phi = 1.28 \). These results for \( \phi \) are in good agreement with estimates obtained by other means.\(^5,7\)

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\(^{7}\)M. E. Fisher and P. Pfeuty (private communication).

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**Magnetic-Ground-State Properties in Praseodymium Single Crystals**

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From hyperfine–specific-heat measurements at very low temperatures we conclude that the ground state in double hcp Pr single crystals must be a magnetically ordered state. Within experimental error the hyperfine specific heat in a single crystal is in agreement with data on polycrystalline material. This is surprising since recent neutron-scattering data in Pr single crystals do not indicate any magnetic order down to 1.7 K, while neutron-scattering data on polycrystalline samples indicated antiferromagnetic order with a Néel temperature of 25 K.

**INTRODUCTION**

The low-temperature form of Pr is known to exhibit the double hcp structure of the ABAC stacking type. Within the first-nearest-neighbor approximation there are 50% sites of cubic point symmetry (A layers) and 50% sites of hexagonal point symmetry (B and C layers). Correspondingly the \( J = 4 \) ground state undergoes an entirely different crystal field splitting in the two sites. The ground state in both sites, however, is expected to be a singlet. Low-field susceptibility\(^1\) as well as resistivity measurements\(^2\) indicate a Néel temperature of 22–23 K in polycrystalline material. In contrast, specific-heat results only show a very weak anomaly around 3.3 K but no \( \lambda \)-type anomaly at 23 K as characteristic of a cooperative magnetic-ordering effect.\(^3,4\) Also, the specific-heat data of various authors differ by more than 30% below 4 K. Neutron-diffraction studies in polycrystals by Cable et al.\(^5\) showed a Néel temperature of 25 K and indicate an average moment of 0.70 \( \mu_B \) on the hexagonal sites only. Recent hyperfine–specific-heat measurements\(^6\) as well as Mössbauer spectroscopy results\(^7\) on a polycrystal of double hcp Pr are also consistent with this average moment. The fact that only the hexagonal sites order\(^8\) is understandable since it takes a minimum ratio of exchange-interaction strength divided by the separation of the first two crystal field levels in order...