PHYSICAL REVIEW VOLUME 176, NUMBER 2 10 DECEMBER 1968

Spherical Model as the Limit of Infinite Spin Dimensionality

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(Received 20 April 1968)

The Berlin-Kac spherical model (or "spherical approximation to the Ising model")

$$\mathcal{H}^{SM} = -J \sum_{\langle ij \rangle} \mu_i \mu_j, \quad \text{with} \quad \sum_{j=1}^{N} u_j^2 = N,$$

is found to be equivalent to the $\nu \to \infty$ limit of the Hamiltonian

$$\mathcal{H}^{(\nu)} = -J \sum_{\langle ij \rangle} \mathbf{S}_i^{(\nu)} \cdot \mathbf{S}_j^{(\nu)},$$

where $\mathbf{S}_j^{(\nu)}$ are isotropically interacting ν-dimensional classical spins.

I. INTRODUCTION

THE Berlin-Kac spherical model[1] has received considerable attention, particularly because it is exactly soluble,[2] and because its solution has led to various ideas concerning the "mathematical mechanism" of phase transitions.[3] The spherical model (SM) Hamiltonian is

$$\mathcal{H}^{SM} = -\tfrac{1}{2} J \sum_{i,j=1}^{N} v_{ij} \mu_i \mu_j, \tag{1a}$$

where the energy of two parallel spins on sites[4] i and j is $-J v_{ij} \mu_i \mu_j$ and the "spins" μ_j are continuous variables subject only to the constraint

$$\sum_{j=1}^{N} \mu_j^2 = N. \tag{1b}$$

Consider now the Hamiltonian[5]

$$\mathcal{H}^{(\nu)} = -\tfrac{1}{2} J \sum_{i,j=1}^{N} v_{ij} \mathbf{S}_i^{(\nu)} \cdot \mathbf{S}_j^{(\nu)}, \tag{2a}$$

where $\mathbf{S}_j^{(\nu)} \equiv [\sigma_1(j), \sigma_2(j), \cdots, \sigma_\nu(j)]$ are ν-dimensional vectors of magnitude $\nu^{1/2}$. Thus the single constraint of the spherical model is replaced by a set of N constraints

$$\sum_{n=1}^{\nu} \sigma_n^2(j) = \nu, \qquad j = 1, 2, \cdots, N. \tag{2b}$$

Although it is perhaps not generally appreciated, it seems clear that $\mathcal{H}^{(\nu)}$ reduces to the $S = \frac{1}{2}$ Ising, classical planar, and classical Heisenberg models for $\nu = 1$, 2, and 3, respectively.

Here we argue that in the limit $\nu \to \infty$, the free energy of $\mathcal{H}^{(\nu)}$ approaches that of the spherical model. This result is of particular current interest (besides the geometrical interpretation it attaches to the spherical model) because of recent evidence[5] that various "critical properties" of $\mathcal{H}^{(\nu)}$ are monotonic functions of ν. Hence the critical properties of the fairly realistic but hopelessly insoluble Heisenberg model (three-dimensional spins) would appear to be bounded on one side by those of the Ising model (one-dimensional spins) and on the other by those of the spherical model (infinite-dimensional spins). Moreover, the spherical model has in the past been interpreted as a soluble approximation to the Ising model, whereas in fact the spherical model would appear to be a much better approximation to the more "realistic" Heisenberg model.

II. EQUIVALENCE OF FREE ENERGIES

The normalized partition function corresponding to $\mathcal{H}^{(\nu)}$ is

$$Q_N^{(\nu)}(K) = Z_N^{(\nu)}(K) / Z_N^{(\nu)}(0), \tag{3}$$

where

$$Z_N^{(\nu)}(K) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} d\sigma_1(1) d\sigma_2(1) \times \cdots d\sigma_\nu(1) d\sigma_1(2) d\sigma_2(2) \cdots d\sigma_\nu(N) \times \prod_{j=1}^{N} [\delta(\nu - \sum_{n=1}^{\nu} \sigma_n^2(j))] \exp[K \sum_{ij} v_{ij} \sum_{n=1}^{\nu} \sigma_n(i) \sigma_n(j)] \tag{4}$$

* Operated with support from the U.S. Air Force.

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[1] For an interesting account of the background of the spherical model, first proposed by M. Kac in 1947, see M. Kac, Phys. Today **17**, 40 (1964).

[2] The exact solution for n.n. interactions is provided by T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952), hereafter referred to as BK.

[3] See, e.g., M. Kac and C. J. Thompson, Proc. Nat. Acad. Sci. **55**, 676 (1966).

[4] The customarily considered "n.n. model" chooses $v_{ij} = 1$ if sites i and j are nearest neighbors and $v_{ij} = 0$ otherwise.

[5] H. E. Stanley, Phys. Rev. Letters **20**, 589 (1968).

and $K\equiv J/2kT$. The N constraints are then represented as

$$\prod_{j=1}^{N}\delta(\nu-\sum_{n=1}^{\nu}\sigma_n^2(j))=\prod_{j=1}^{N}\frac{K}{2\pi i}\int_{-i\infty}^{i\infty}dt_j \times\exp\{Kt_j[\nu-\sum_{n=1}^{\nu}\sigma_n^2(j)]\} \quad (5)$$

and we obtain

$$Z_N^{(\nu)}(K)=\left(\frac{K}{2\pi i}\right)^N\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}d\sigma_1(1)\cdots d\sigma_\nu(N) \times\int_{-i\infty}^{i\infty}\cdots\int_{-i\infty}^{i\infty}dt_1\cdots dt_N\exp(\nu K\sum_j t_j) \times\prod_{n=1}^{\nu}\exp\{-K\sum_{ij}[t_j\delta_{ij}-v_{ij}]\sigma_n(i)\sigma_n(j)\}. \quad (6)$$

We next interchange the order of the $d\sigma_n(j)$ and dt_j integrations following the method used by BK[2] in connection with their Eq. (C3).[6] The $d\sigma_n(j)$ integrations then factorize, with the result

$$Z_N^{(\nu)}(K)=\left(\frac{K}{2\pi i}\right)^N\int_{\alpha-i\infty}^{\alpha+i\infty}\cdots\int_{\alpha-i\infty}^{\alpha+i\infty}dt_1\cdots dt_N \times\exp(\nu K\sum_j t_j)[I(K,\{t_j\})]^\nu, \quad (7)$$

where

$$I(K,\{t_j\})\equiv\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}d\sigma_n(1)\cdots d\sigma_n(N) \times\exp[-K\sum_{ij}(t_j\delta_{ij}-v_{ij})\sigma_n(i)\sigma_n(j)]. \quad (8)$$

The evaluation of the integral in Eq. (8) is straightforward, and we find

$$I(K,\{t_j\})=(\pi/K)^{N/2}[\Delta(\{t_j\})]^{-1/2}, \quad (9)$$

where $\Delta(\{t_j\})$ is the determinant of the quadratic form $\sum_{ij}(t_j\delta_{ij}-v_{ij})\sigma_n(i)\sigma_n(j)$. On substituting Eq. (9) into Eq. (7), we finally obtain

$$Z_N^{(\nu)}(K)=\left(\frac{K}{2\pi i}\right)^N\left(\frac{\pi}{K}\right)^{\nu N/2}\int_{\alpha-i\infty}^{\alpha+i\infty}\cdots\int_{\alpha-i\infty}^{\alpha+i\infty}dt_1\cdots dt_N \times\exp[\nu F(K,\{t_j\})], \quad (10)$$

with

$$F(K,\{t_j\})\equiv K\sum_j t_j-\tfrac{1}{2}\ln\Delta(\{t_j\}). \quad (11)$$

[6] To apply the BK "trick" to Eq. (6), we set

$$1=\exp[K\sum_{j=1}^{N}b_j(\nu-\sum_{n=1}^{\nu}\sigma_n^2(j))]$$

which is true for any values of the numbers b_j because of the constraints (5). We choose $b_j=\alpha[j=1,2,\cdots,N]$, where α is a sufficiently large positive real number that the quadratic form $\Sigma_{ij}[(t_j+\alpha)\delta_{ij}-v_{ij}]\sigma_n(i)\sigma_n(j)$ is positive definite. Finally, Eq. (7) is obtained by the change of integration variable $t_j\rightarrow t_j+\alpha$.

The requirement that $F(K,\{t_j\})$ be stationary leads to the set of conditions

$$K=\tfrac{1}{2}((\partial/\partial t_l)[\ln\Delta(\{t_j\})])_{t_s}, \qquad l=1,2,\cdots,N. \quad (12)$$

Proceeding in the customary fashion,[7] we obtain the expression

$$K=\tfrac{1}{2}N^{-1}\sum_{\mathbf{q}}[\lambda_{\mathbf{q}}(K,t_s)]^{-1}, \quad (13)$$

with

$$\lambda_{\mathbf{q}}(K,t_s)=t_s-\hat{v}_{\mathbf{q}} \quad (14)$$

and

$$\hat{v}_{\mathbf{q}}=N^{-1}\sum_{ij}v_{ij}\exp[i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)]. \quad (15)$$

For a $[d]$-dimensional "hypercubical" (linear chain, square, simple cubic, $\cdots$) lattice with nonzero interactions only between spins on nearest-neighbor (n.n.) sites,[4] Eq. (13) becomes

$$2K=\langle[t_s-2\sum_{m=1}^{d}\cos\omega_m]^{-1}\rangle, \quad (16)$$

where the brackets indicate the "average"

$$\langle g(\{\omega_m\})\rangle\equiv\pi^{-d}\int_0^\pi\cdots\int_0^\pi d\omega_1\cdots d\omega_d g(\{\omega_m\}). \quad (17)$$

The analogous expression determining the spherical model stationary point z_s is [cf. BK, Eq. (C23)]

$$4K=\langle[z_s-\sum_{m=1}^{d}\cos\omega_m]^{-1}\rangle, \quad (18)$$

thus $t_s=2z_s$.

Next expand $F(K,\{t_j\})$ about the stationary points $\{t_s\}$,

$$F(K,\{t_j\})=F(K,\{t_s\})+\frac{1}{2!}\sum_{m,n=1}^{N}\left(\frac{\partial^2F}{\partial t_m\partial t_n}\right)_{t_s} \times(t_m-t_s)(t_n-t_s)+\cdots. \quad (19)$$

[7] That the stationary values of all the variables t_j are identical is explained by E. Helfand and J. S. Langer, Phys. Rev. **160**, 437 (1967). These authors treated critical correlations (for $T\simeq T_c$) in the Ising model and were thereby led to consider Eq. (10) for the case $\nu=1$. They remarked that the integrand of Eq. (10) for the Ising model is stationary at $\{t_s\}$ (as indeed it is for *all* values of ν), but in their Eq. (2.14) they imply that the spherical-model partition function is given, "except for some simple normalization terms," by the value of the integrand evaluated at t_s. We note that there appears to be no way of obtaining suitable "normalization terms" such that the right-hand side of their Eq. (2.14) equals the left-hand side. One might imagine that they are referring to a normalization term such as $Z_N^{(\nu)}(0)$ as given by Eq. (23) of the present paper; however for the Ising model, $Z_N^{(1)}(0)=1$. [Incidentally, it is in fact Eq. (23) when evaluated not for $\nu=1$ but rather in the limit $\nu\rightarrow\infty$ which provides precisely the required normalization for our $\nu\rightarrow\infty$ result, Eq. (27).] Helfand and Langer were, to the best of our knowledge, the first to apply saddle-point methods to integrals such as Eq. (10). Such integrals arose (in their work as well as in ours) from the idea of expressing the Ising model partition function not as a sum but rather as an integral, an idea first exploited (we believe) by E. W. Montroll and T. H. Berlin, Commun. Pure Appl. Math. **4**, 23 (1951).

We then factor $\nu F(K, \{t_s\})$ out of the integrand, calling the remaining integral

$$R \equiv \left(\frac{K}{2\pi i}\right)^N \int_{\alpha-i\infty}^{\alpha+i\infty} \cdots \int_{\alpha-i\infty}^{\alpha+i\infty} dt_1 \cdots dt_N$$

$$\times \exp\left[\frac{1}{2!}\nu \sum_{m,n=1}^{N} \left(\frac{\partial^2 F}{\partial t_m \partial t_n}\right)_{t_s} (t_m - t_s)(t_n - t_s) + \cdots \right]. \quad (20)$$

Thus, from Eq. (10),

$$\ln Z_N^{(\nu)}(K) = \tfrac{1}{2}\nu N \ln(\pi/K) + \nu F(K, \{t_s\}) + \ln R. \quad (21)$$

From Eq. (3), the limiting free energy $\psi^{(\infty)}$ is related to $Z_N^{(\nu)}(K)$ by

$$-\beta\psi^{(\infty)} \equiv \lim_{\nu, N\to\infty} (\nu N)^{-1} \ln[Z_N^{(\nu)}(K)/Z_N^{(\nu)}(0)], \quad (22)$$

where $\beta \equiv (kT)^{-1}$ and

$$Z_N^{(\nu)}(0) = [(\nu\pi)^{\nu/2}/\nu\Gamma(\tfrac{1}{2}\nu)]^N, \quad (23)$$

as is easily seen by the above methods. On using Stirling's asymptotic expansion of the Γ function in Eq. (23) and then substituting Eqs. (21) and (23) into Eq. (22), we have

$$-\beta\psi^{(\infty)} = -\tfrac{1}{2} - \tfrac{1}{2}\ln 2K + (1/N)F(K, \{t_s\}) + \lim_{\nu, N\to\infty} (\nu N)^{-1} \ln R. \quad (24)$$

The last term on the right-hand side of Eq. (24) can be shown to be zero.[8] Now, $F(K, \{t_s\}) = NKt_s - \tfrac{1}{2}\ln\Delta(\{t_s\})$ from Eq. (11), and

$$\ln\Delta(\{t_s\}) = \ln 2^N + \ln |\tfrac{1}{2}t_s\delta_{ij} - \tfrac{1}{2}v_{ij}| = N\ln 2 + Nf_d(z_s), \quad (25)$$

where $t_s = 2z_s$ and

$$f_d(z_s) \equiv \langle \ln[z_s - \sum_{m=1}^{d} \cos\omega_m] \rangle, \quad (26)$$

exactly as in BK, Eq. (C12). We finally obtain

$$-\beta\psi^{(\infty)} = -\tfrac{1}{2} - \tfrac{1}{2}\ln 4K + 2Kz_s - \tfrac{1}{2}f_d(z_s), \quad (27)$$

which is precisely BK, Eq. (C11).

III. DISCUSSION

The above argument (that the free energy of a system of isotropically-interacting ν-dimensional classical spins approaches, in the limit $\nu \to \infty$, the free energy calculated by Berlin and Kac for the spherical model) is supported by various other evidence, among which we mention the following:

(a) For all lattices the first 10 terms of the high-temperature expansions of the susceptibility and free energy of $\mathcal{H}^{(\nu)}$ agree, on taking the limit $\nu \to \infty$, with those calculated for the spherical model.[5] Thus, if the last term on the right-hand side of Eq. (24) were not zero, for example, its leading term in $1/T$ would have to be of order $(1/T)^{11}$ or smaller.

(b) For the [1]-dimensional linear-chain lattice we can solve exactly for the free energy $\psi^{(\nu)}$ for arbitrary ν without needing to consider an N-fold integration. We find

$$-\beta\psi^{(\nu)} = (1/\nu)\ln[(\nu K)^{1-\nu/2}\Gamma(\tfrac{1}{2}\nu)I_{\nu/2-1}(2\nu K)], \quad (28)$$

where $I_n(x)$ are the modified Bessel functions of the first kind. Thus, on taking the limit $\nu \to \infty$,[9] we obtain

$$-\beta\psi^{(\infty)} = -\tfrac{1}{2} + \tfrac{1}{2}(1+16K^2)^{1/2} - \tfrac{1}{2}\ln\tfrac{1}{2}[1+(1+16K^2)^{1/2}], \quad (29)$$

which is the same result as obtained by BK, Eq. (C18). The fact that ψ^{SM} is explicitly and rigorously given by $\lim_{\nu\to\infty}\psi^{(\nu)}$ for a [1]-dimensional lattice of

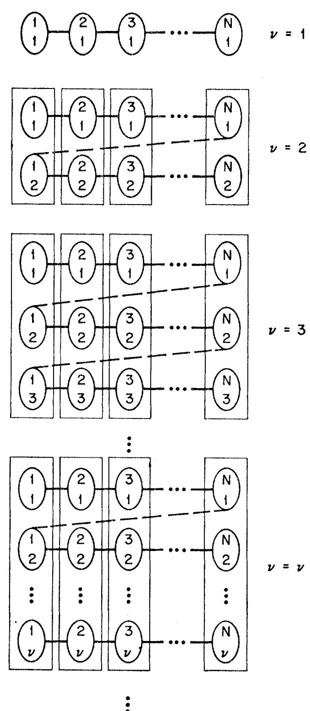

FIG. 1. Model of a linear chain of N ν-dimensional classical spins interacting isotropically with one another via the Hamiltonian $\mathcal{H}^{(\nu)}$. Each oval with j at the top and n at the bottom represents the nth Cartesian component $\sigma_n(j)$ $(n=1, 2, \cdots, \nu)$ of the jth spin $\mathbf{S}_j^{(\nu)}$ $(j=1, 2, \cdots, N)$. The ovals interact with their (horizontal) nearest neighbors via the exchange parameter J (shown by heavy solid lines); they also "interact" with their (vertical) mates via the *constraints* $\delta(\nu - \sum_{n=1}^{\nu}\sigma_n^2(j))$ (as indicated by the thin-lined rectangles). If we now assume that there is also an interaction between the scalar spins $\sigma_n(N)$ and $\sigma_{n+1}(1)$ (as indicated by the heavy dashed lines), then we obtain, in the limit $\nu \to \infty$, an N-spherical model whose thermodynamic functions (according to Ref. 11) are identical with those of the ordinary BK spherical model.

[8] R. N. Lewis, in *Asymptotic Solutions of Differential Equations and Their Applications*, edited by C. H. Wilcox (John Wiley & Sons, Inc., New York, 1964), p. 53 [also obtainable on request from the Courant Institute of Mathematical Sciences, New York University as NYU Research Report No. EM-197) (unpublished)].

[9] The relevant asymptotic expansion for modified Bessel functions of the first kind when both the argument and the order approach infinity is developed in G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, London, 1958), Chap. 8.

course proves nothing about [2]- and [3]-dimensional lattices.[10]

(c) We can present an intuitive explanation of our result based upon a recent theorem that the thermodynamic functions of all "m-spherical" models are equal to those of the BK spherical model.[11] Here "m-spherical model" refers to a model in which the full set of lattice sites is partitioned into m distinct subsets (or "sublattices") R_α [$\alpha=1, 2, \cdots, m$] with $\mathfrak{N}_1, \mathfrak{N}_2, \cdots, \mathfrak{N}_m$ sites belonging to each sublattice. With each lattice site is associated a scalar spin μ_j, and with each sublattice R_α is associated the constraint

$$\sum_{j=1}^{N_\alpha} \mu_j^2 = \mathfrak{N}_\alpha.$$

The theorem then states that providing the number of sites belonging to each sublattice tends to infinity (i.e., $\mathfrak{N}_\alpha \to \infty$ for $\alpha=1, 2, \cdots, m$), we recover the thermodynamic functions of the ordinary BK spherical model (or 1-spherical model). Now the sublattices need not be contiguous, as illustrated for the case of the linear-chain lattice in Fig. 1. Here the thin-lined rectangles enclose each "sublattice" R_α, where $\alpha=1, 2, \cdots, N$ (i.e., $m\equiv N$ here) and each sublattice is composed of ν scalar "spins" $\sigma_n(\alpha)$ ($n=1, 2, \cdots, \nu$). If we assume that each heavy solid line as well as the heavy dashed line represents a n.n. interaction, then the theorem will apply in the limit as $\nu\to\infty$. Now our model Hamiltonian $\mathcal{H}^{(\nu)}$ is obtained by breaking all the dashed lines which, for n.n. exchange interactions, represents an energy change of order $1/N$, so that one might expect that the theorem would continue to hold.

In conclusion, we should like to supplement the remarks made in Sec. I concerning why our result may prove to be of some utility.

(a) A knowledge of the properties of the model Hamiltonian $\mathcal{H}^{(\nu)}$ in the limit $\nu\to\infty$ provides one with an "anchor point," since $\mathcal{H}^{(\nu)}$ is not soluble for other values of ν (except for the linear chain lattice—and for [2]-dimensional lattices, provided that $\nu=1$). For example, various approximation techniques (such as extrapolation from high-temperature expansions, Green's-function decoupling schemes, etc.) can be "tested" on the spherical model, for which the *exact* values of the various critical properties are known. It is also feasible to calculate numerically 100 terms in the various expansions for the spherical model, and the fact that the *correct* values for the various critical properties are indicated[12] tends to discredit the frequently made charges that the regularity observed in the first 10 or so terms of the expansions available[5] for general ν is misleading or spurious.[13]

(b) An asymptotic expansion of the free energy for large ν might provide a good approximation to the Heisenberg model ($\nu=3$), and could provide some insight into various (as yet unsolved) problems for systems of two- and three-dimensional spins—such as the question of whether there exists any sort of "phase transition"[14] for [2]-dimensional lattices when ν is small [apart from the conventional ($M\neq0$) transition for $\nu=1$]. A treatment of some of the effects found when ν is large but not infinite has been carried out very recently by Helfand.[15]

ACKNOWLEDGMENTS

I wish to thank Professor Norman Bleistein, Dr. Eugene Helfand, and Dr. Thomas A. Kaplan for valuable advice and stimulating discussions. I have also benefited from comments by several workers who attended the statistical-mechanics meeting of the Belfer School of Science, where I presented some of the above results. Thanks are also due to Dr. Herbert J. Zeiger and Dr. Marvin M. Litvak for their encouragement and support throughout the course of this work. The point made in the Appendix arose from remarks of E. Helfand. Finally, I wish to thank Professors Mark Kac and Robert M. Mazo for a critical reading of the manuscript.

APPENDIX: INABILITY TO RULE OUT DISCONTINUOUS BEHAVIOR OF CRITICAL INDICES

The above argument that

$$\lim_{\nu\to\infty}\{\psi^{(\nu)}(T)\}=\psi^{\text{SM}}(T) \tag{A1}$$

is valid only for $T\neq T_c$; therefore the same argument cannot be used to prove that, e.g.,

$$\lim_{\nu\to\infty}\{\alpha^{(\nu)}\}=\alpha^{\text{SM}} \tag{A2}$$

[10] A more detailed treatment of the linear chain is presented in H. E. Stanley, Proceedings of the International Conference on Statistical Mechanics (to be published in J. Phys. Soc. Japan).

[11] G. V. Bettoney and R. M. Mazo (unpublished). I wish to thank Professor M. E. Fisher for calling this work to my attention and Professor Robert M. Mazo for sending me an unpublished report.

[12] H. E. Stanley (unpublished) and Ref. 10.

[13] Hitherto the most convincing counterargument to these "charges" was that the 10–15 available terms for the [2]-dimensional Ising model appeared to extrapolate to the exact critical values. Thus the availability of 100 terms for both [2]- and [3]-dimensional lattices for $\nu=\infty$ would seem to considerably strengthen the argument based upon $\nu=1$ only. Moreover, the form of the various thermodynamic functions at the critical temperature has always been open to question, since there is no firm evidence supporting the commonly-assumed "power-law" divergences (for example, it has not been rigorously proved, even for the [3]-dimensional Ising model, that the susceptibility diverges with a simple power law, let alone that the "critical exponent" $\gamma^{(1)}$ is 5/4). For $\nu=\infty$ one can see that the susceptibility for [3]-dimensional lattices does diverge with a power law, and that $\gamma^{(\infty)}=2$. Furthermore, the estimated values of $\gamma^{(\nu)}$ for other values of ν are very nearly given by the smoothly-varing function $\gamma^{(\nu)}=1+\tanh[\frac{1}{16}(\nu+3)]$.

[14] Indeed, since for $\nu>1$ the spontaneous magnetization is zero for all temperatures $T>0$, the phase transitions for two-dimensional lattices indicated by high-temperature expansions would have to be to a low-temperature phase [see, e.g., H. E. Stanley and T. A. Kaplan, Phys. Rev. Letters **17**, 913 (1966)] with no infinite-range order M, yet with sufficient long-range order that χ diverges to infinity.

[15] E. Helfand (to be published).

for the sequence of specific heat exponents $\alpha^{(\nu)}$. The reason is of course that the "critical indices" (such as $\alpha^{(\nu)}$) are defined as the $T\rightarrow T_c$ limit of certain functionals $f[\psi^{(\nu)}(T)]$, and we cannot rule out the possibility that

$$\lim_{\nu\to\infty}\{\lim_{T\to T_c} f[\psi^{(\nu)}(T)]\}\neq \lim_{T\to T_c} f[\psi^{SM}(T)]. \quad (A3)$$

Although the terms in the various high-temperature expansions would have to depart from their apparently smooth variation with ν at *some* order if the critical indices were to behave discontinuously as a function of ν, the fact that there is absolutely no indication of this through order $1/T^{10}$ does not *prove* anything one way or the other.

PHYSICAL REVIEW VOLUME 176, NUMBER 2 10 DECEMBER 1968

Magnetic Structures of Er_2O_3 and Yb_2O_3†

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The magnetic structures of Er_2O_3 and Yb_2O_3 have been determined by analysis of neutron diffraction data on powders and single crystals. Noncollinear antiferromagnetic structures were found, with the moment direction related to the local symmetry axis. For Er_2O_3, the moment on the C_2 site is $(5.36\pm0.08)\mu_B$ and at the C_{3i} site the moment is $(6.06\pm0.23)\mu_B$. For Yb_2O_3, the corresponding moments are $(1.86\pm0.06)\mu_B$ and $(1.05\pm0.06)\mu_B$. The Néel points are 3.4°K for Er_2O_3 and 2.3°K for Yb_2O_3. Calculations of the dipole-dipole energies for the observed structures indicate that the dipole forces are not sufficient to explain the structures. The dependence of the long-range magnetic order on the reduced temperature is the same in both systems. Good agreement with this temperature dependence was obtained by assuming a biquadratic exchange interaction and making a simple molecular-field approximation.

I. INTRODUCTION

THE rare-earth oxides form an interesting class of magnetic materials because of their weak magnetic interactions. For example, the Néel points of Er_2O_3 and Yb_2O_3 are 3.4 and 2.3°K, respectively. These temperatures are low enough that the magnetic dipole interaction must be considered a possible cause of the magnetic order. One of the objectives of this investigation was to evaluate the importance of the dipole interaction by deducing the magnetic structure from neutron diffraction data, calculating the dipolar interaction energy of this structure, and comparing the result with the observed Néel temperature. Another implication of a low Néel point is that the magnetic interaction, whatever its origin, is a small perturbation compared to the crystal-field interaction. The low-temperature magnetic properties, therefore, should be strongly influenced by the crystal field. If the magnetic interaction is very weak compared to the energy of the first excited crystal-field level, the ordered moment should be a property of the crystal-field ground state. A somewhat stronger magnetic interaction will mix the crystal-field states, as discussed by Bleaney,[1] leading to a new ground state with a moment that is a function of the strength of the magnetic interaction.

The intermediate case, in which the ground-state wave function is dependent on the strength of the magnetic interaction, can lead to unusual magnetic behavior as a function of temperature and applied field. For example, if the dominant coupling mechanism is superexchange the interatomic exchange constants are related to the rare-earth-oxygen overlap integrals. But as the degree of magnetic order increases, these overlap integrals may change because the rare-earth ground state is changing. Thus the interatomic exchange parameters are not constant, but become functions of temperature. Applied fields can also change the degree of admixture of the crystal-field states. This effect, in addition to the weak magnetic interaction, means that the magnetic structures can be easily influenced by applied fields. As an additional complication, we will see that there is some evidence indicating that biquadratic exchange may be important.

Neutron diffraction studies have been made on single crystals and powders of Er_2O_3 and Yb_2O_3. The expected complex nature of the temperature and field dependence of the magnetic structures has been fully realized.

These materials all have the bixbyite[2] structure. There are 32 rare-earth ions and 48 oxygens in a cubic unit cell with lattice constant of about 10.5 Å. The space group is $Ia3-T_h^7$. Twenty-four of the rare earths are on sites with twofold rotational symmetry (C_2), and eight are on sites with threefold rotary inversion symmetry (C_{3i}). There is one adjustable position parameter for the C_2 sites, none for the C_{3i} sites, and three for the oxygen sites. The oxygen coordination around the two rare-earth sites is shown in Fig. 1. For the C_2 site, the oxygens fall almost on the corners of a cube with the rare earth at the center and with two missing oxygens along a face diagonal. The twofold axis is perpendicular to this face diagonal. One of the symmetry elements of the space group is the body-centered translation, so that there are two C_2

† Research sponsored by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation.
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[1] B. Bleaney, Proc. Roy. Soc. (London) **A276**, 19 (1963).
[2] L. Pauling and M. D. Shappell, Z. Krist. **75**, 128 (1930).