One-Dimensional Order-Disorder Model Which Approaches a Second-Order Phase Transition*

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The calculation of the partition function for a simple one-dimensional order-disorder model is reduced to the solution of a certain functional equation. This equation is solved rigorously and it is shown that in the limit of indefinitely long-range interactions the model exhibits a finite discontinuity in the specific heat.

1. INTRODUCTION

As many authors have pointed out,[1] the rigorous deduction of the existence of a phase transition and determination of its properties from first principles is immensely difficult for realistic models of physical systems. We study in this paper a simplified model of a one-dimensional system which can manifest varying degrees of order. It is an extension of the well-known "Ising" model. We allow each spin to interact with all spins in the system, the interaction energy dropping off exponentially with the separation distance. We find that as the range of the interaction increases indefinitely, the maximum slope of the specific heat curve also increases indefinitely. In the limit of infinitely long-range interaction, the system manifests a second-order phase transition of the same type as the lambda transition of liquid He^4; that is, the specific heat increases rapidly with temperature until a critical temperature is reached, and then it drops discontinuously. The existence of a transition in this limit can be understood qualitatively in terms of the possibility of existence of long-range order. When the range of interaction is finite, the existence of a finite number of consecutive "wrong" spins suffices to separate two regions of oppositely directed perfect order. As, for any temperature different from zero, there is a definite probability, which does not go to zero with increasing system size, that any finite number of consecutive spins will be "wrong," long-range order cannot exist. However, the longer the range, the smaller the probability. In the limit of infinitely long-range interactions, this probability goes to zero for sufficiently low temperatures and hence in that limit long-range order can exist.

In Sec. 2 we show how the calculation of the partition function may be reduced to the solution of a certain eigenvalue, functional equation. In Sec. 3 we solve this equation for any finite range of interaction. In Sec. 4 we discuss the behavior in the neighbor of the Ising model limit—very short-range interactions. In the last section we discuss the limit as the range of interaction increases indefinitely and deduce the existence of a second order phase transition in this limit. Needless to say, for a long but finite range, the specific heat curve is very difficult to distinguish experimentally from that for infinitely long-range interactions. We discuss the Bragg-Williams approximation in an Appendix and point out that while it is similar to the limit of indefinitely long-range forces for this model, it is not identical with it.

2. REDUCTION TO A FUNCTIONAL EQUATION

Let us consider a one-dimensional array of N spins (ν_j). We shall treat it in the "Ising" approximation; that is, we consider only the z component of the spins. Thus, we shall treat the spins as scalars and allow them to assume only the values ± 1. We shall *not* restrict ourselves to nearest neighbor interactions only, but assume that the spin-spin interaction energy decreases exponentially with the distance separating the spins. Thus, if we number the spins (assumed to be equally spaced), then the interaction energy between the jth and kth spins will be proportional to

$$\nu_j\nu_k \exp(-\gamma|j-k|).$$

For convenience, let us set $e^{-\gamma}=r$ and let rJ be the nearest-neighbor exchange integral. We restrict $0\leqq r<1$, for exponentially decreasing interactions.

If we now sum over all pair interactions, the total spin-spin interaction energy of the array will be

$$-J\sum_{j=1}^{N-1}\sum_{k=j+1}^{N} r^{k-j}\nu_j\nu_k. \tag{2.1}$$

To facilitate the subsequent discussion, let us introduce the relative spin between nearest-neighbor spins:

$$\begin{aligned}&\mu_j=\nu_j\nu_{j+1}, \quad j=1, N-1\\ &\mu_N=\nu_N.\end{aligned} \tag{2.2}$$

If we make use of the fact that $\nu_j^2=1$, we may rewrite the product $\nu_j\nu_k(k>j)$ in terms of the μ_j as

$$\begin{aligned}\nu_j\nu_k&=\nu_j\nu_{j+1}\nu_{j+1}\nu_{j+2}\nu_{j+2}\cdots\nu_{k-1}\nu_{k-1}\nu_k\\ &=\prod_{i=j}^{k-1}\mu_i.\end{aligned}$$

If we rewrite (2.1) in terms of the μ's and let i be the k

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[1] See, for instance, L. Van Hove, Revs. Modern Phys. **29**, 200 (1957).

of (2.1) minus j, then the energy becomes

$$-J\sum_{j=1}^{N-1}\sum_{i=1}^{N-j}\left(\prod_{k=j}^{i+j-1}\mu_k r\right). \tag{2.3}$$

If we denote the interaction energy divided by $(-J)$ of spin j with all spins of higher location number by y_j, then

$$y_j=\sum_{k=j+1}^{N} r^{k-j}\nu_j\nu_k=\sum_{i=1}^{N-j}\left(\prod_{k=j}^{i+j-1}\mu_k r\right). \tag{2.4}$$

We shall now show that the y_j satisfy a simple recursion relation

$$\begin{aligned} y_j&=\mu_j r+\sum_{i=2}^{N-j}\left(\mu_j r\prod_{k=j+1}^{i+j-1}\mu_k r\right)\\ &=\mu_j r\left[1+\sum_{\omega=1}^{N-(j+1)}\left(\prod_{k=j+1}^{\omega+(j+1)-1}\mu_k r\right)\right], \end{aligned} \tag{2.5}$$

or

$$y_j=\mu_j r(1+y_{j+1}),\quad y_{N-1}=\mu_{N-1}r. \tag{2.6}$$

By comparing (2.3) with (2.4) we see that the energy may be written in terms of the y_j as simply

$$-J\sum_{j=1}^{N-1} y_j.$$

The standard partition function for this system is

$$\begin{aligned} Z_N(y_N)&=\sum_{\{\nu_j\}}\exp[-E(\nu_j)/kT]\\ &=\sum_{\{\mu_j\}}\exp[(J/kT)\sum_{j=1}^{N-1} y_j], \end{aligned} \tag{2.7}$$

where the summation goes over all 2^{N-1} possible configurations of the first $N-1$ spins.

In order to evaluate Z as a function of T and r, let us introduce

$$\begin{aligned} &x_j=(1-r)y_j/r,\quad j=1,N-1\\ &K=Jr/[(1-r)kT],\\ &f_j(x_j)=2Z_j(x_j)\Big/\int_{-1}^{+1}Z_j(x_j)dx_j, \qquad (2.8)\\ &\lambda_j=\int_{-1}^{+1}Z_{j+1}(x_j)dx_j\Big/\int_{-1}^{+1}Z_j(x_{j-1})dx_{j-1}, \end{aligned}$$

where Z_j is defined to be the partition function for the first $j-1$ spins, as in (2.7), clearly depends only on $x_j(Z_1\equiv 1)$. It is to be noted that holding K instead of rJ fixed while varying r corresponds to holding the maximum possible interaction energy fixed instead of the nearest-neighbor interaction energy. This distinction is important in the limit as $r\to 1$. We shall evaluate $f_{j+1}(x_{j+1})$ in terms of f_j. Now

$$Z_{j+1}(x_{j+1})=\sum_{\mu_j=\pm 1}\exp[Kx_j]Z_j(x_j), \tag{2.9}$$

or

$$\begin{aligned} \lambda_j f_{j+1}(x_{j+1})=\sum_{\mu_j=\pm 1}&\exp[\mu_j K(1-r+rx_{j+1})]\\ &\times f_j(\mu_j(1-r+rx_{j+1})). \end{aligned} \tag{2.10}$$

Thus, dropping the subscript on x_{j+1} and summing over μ_j, we obtain

$$\begin{aligned} \lambda_j f_{j+1}(x)=&\exp[K(1-r+rx)]f_j(1-r+rx)\\ &+\exp[-K(1-r+rx)]f_j(-1+r-rx), \end{aligned} \tag{2.11}$$

and, for the partition function, taking account the slightly different dependence on μ_{N-1} and μ_N, we obtain

$$Z_{N+1}(0)=2[\prod_{j=1}^{N-1}\lambda_j]f_N(0). \tag{2.12}$$

If the λ_j and f_j tend to a limit, as j increases indefinitely, then the partition function per spin is

$$\ln[z(K)]=\lim_{N\to\infty}\{[\ln Z_{N+1}(0)]/N\}=\ln\lambda, \tag{2.13}$$

where λ is the largest eigenvalue of the equation

$$\begin{aligned} \lambda f(x)=&\exp[K(1-r+rx)]f(1-r+rx)\\ &+\exp[-K(1-r+rx)]f(-1+r-rx). \end{aligned} \tag{2.14}$$

As we shall see in the next section, the iteration process prescribes a unique solution for (2.14).

We further note that if $-1\le x\le+1$, then $|1-r+rx|\le 1$ so that a knowledge of $f(x)$ over the unit interval suffices. The ends of the unit interval correspond to the least upper bound and greatest lower bound for the energy of interaction of a single spin with all the spins of higher index numbers.

3. SOLUTION OF THE FUNCTIONAL EQUATION

It follows by direct substitution and comparison that if $f(x)$ is a solution of (2.14), then

$$f\left(y-\frac{1-r}{r}\right)=f\left(-y-\frac{1-r}{r}\right). \tag{3.1}$$

Hence let us consider

$$g(y)=f\left(y-\frac{1-r}{r}\right)=g(-y). \tag{3.2}$$

Equation (2.14) then becomes

$$\lambda g(y)=e^{+r\,Ky}g\left(\frac{1-r}{r}+ry\right)+e^{-r\,Ky}g\left(\frac{1-r}{r}-ry\right). \tag{3.3}$$

If one iterates Eq. (3.3) in the manner prescribed by (2.11) starting with $g_1\equiv 1$, then, adopting the normalization $g_j(0)=1$ instead of (2.8), it is readily apparent for all g_j that (i) $g_j(x)$ possess a power series expansion

which converges absolutely for all x, and (ii) if $g_j(x)$ is thought of as a double-power series in K and x, no terms occur in which the power of x exceeds that of K. Therefore, we shall seek a solution for $g(y)$ and λ of the form

$$g(y)=\sum_{n=0}^{\infty}\{\sum_{m=0}^{[n/2]}a_{nm}y^{2m}\}K^n,$$
$$\lambda=\sum_{j=0}^{\infty}\lambda_j K^j, \tag{3.4}$$

where $[a]$ denotes the greatest integer not exceeding a.

Kac[2] has shown that λ is also the largest eigenvalue of an integral equation whose kernel is of the Hilbert-Schmidt type. As pointed out by him, one may easily deduce from his integral equation that there is no phase transition in the model. More precisely, it is easy to show that $\lambda(K)$ is analytic for K real. This result means, in particular, that $\lambda(K)$ has a power series representation about $K=0$.

If we substitute (3.4) into Eq. (3.3) we will obtain, by equating coefficients, a sequence of equations for the a_{nm} and λ_j of (3.3). On performing the substitution, we find

$$\sum_{j=0}^{\infty}\lambda_j K^j\sum_{n=0}^{\infty}\{\sum_{m=0}^{[n/2]}a_{nm}y^{2m}\}K^n=\sum_{j=0}^{\infty}(rKy)^j(j!)^{-1}\sum_{n=0}^{\infty}K^n\sum_{m=0}^{[n/2]}a_{nm}\sum_{k=0}^{2m}\binom{2m}{k}\left(\frac{1-r}{r}\right)^{2m-k}(ry)^k$$
$$+\sum_{j=0}^{\infty}(-rKy)^j(j!)^{-1}\sum_{n=0}^{\infty}K^n\sum_{m=0}^{[n/2]}a_{nm}\sum_{k=0}^{2m}\binom{2m}{k}\left(\frac{1-r}{r}\right)^{2m-k}(-ry)^k, \tag{3.5}$$

where $\binom{2m}{k}$ denotes the standard binomial coefficients. On equating the coefficients of K^ν, we obtain

$$\sum_{j=0}^{\nu}\lambda_j\sum_{m=0}^{[(\nu-j)/2]}a_{\nu-j,m}y^{2m}=\sum_{j=0}^{\nu}(ry)^j(j!)^{-1}\sum_{m=0}^{[(\nu-j)/2]}a_{\nu-j,m}\sum_{k=0}^{2m}\binom{2m}{k}\left(\frac{1-r}{r}\right)^{2m-k}(ry)^k$$
$$+\sum_{j=0}^{\nu}(-ry)^j(j!)^{-1}\sum_{m=0}^{[(\nu-j)/2]}a_{\nu-j,m}\sum_{k=0}^{2m}\binom{2m}{k}\left(\frac{1-r}{r}\right)^{2m-k}(-ry)^k, \tag{3.6}$$

and, finally equating the coefficients of y^μ (μ is automatically even as terms in odd powers of y cancel identically), we have

$$\sum_{j=0}^{\nu-\mu}a_{\nu-j,\mu/2}\lambda_j=2\sum_{j=0}^{\mu}\frac{r^{2\mu-j}}{j!(1-r)^{\mu-j}}\times\sum_{m=[(\mu-j+1)/2]}^{[(\nu-j)/2]}a_{\nu-j,m}\binom{2m}{\mu-j}\left(\frac{1-r}{r}\right)^{2m}. \tag{3.7}$$

On setting $\mu=0$, $\nu=0$, we obtain $\lambda_0=2$. Similarly, $\lambda_1=a_{1,0}=0$. For $\mu=[\nu/2]$, $\nu\geq 2$, we obtain

$$\lambda_\nu=2\sum_{m=1}^{[\nu/2]}a_{\nu,m}\left(\frac{1-r}{r}\right)^{2m}. \tag{3.8}$$

Equation (3.7) may be solved directly for all the $a_{\nu,m}$ in terms of the $a_{\omega,m}$ and λ_ω for $\omega<\nu$ by setting $\mu=[\nu/2]-2$, $[\nu/2]-4$, $\cdots$, 0 successively. This procedure *uniquely* determines the λ_ν and $a_{\nu,m}$. Since the series for $\lambda(K)$ is known to converge for K sufficiently small and

$$\lambda(K)=2g\left(\frac{1-r}{r}\right),\quad [g(0)\equiv 1],$$

it follows that our expansion of $g(y)$ must also converge for the same values of K and $|y|\leq R$, $R\geq(1-r)/r$.

Another procedure to obtain the solution is to iterate Eq. (2.14) over the range $-1\leq x\leq 1$, starting with $f(x)=1.0$. This method may be easily done numerically, and may be used when the function cannot be evaluated conveniently from the power series. We have programmed it for the IBM 704. The range between -1 and $+1$ was divided into N equally spaced intervals and λf_{n+1} at the $N+1$ points, -1, $-1+2/N$, $-1+4/N$, $\cdots$, $+1$ was computed from f_n by use of linear interpolation and Eq. (2.14). The coefficients in the power series expansions through the 50th power of K were also computed for $\lambda(K)$ and $f(x)$ by way of a partial

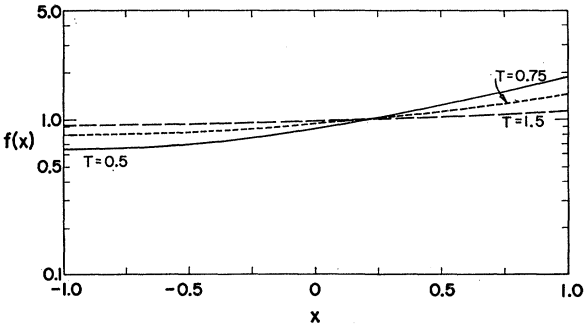

FIG. 1. Probability envelopes for several values of temperature for antiferromagnetic type interactions with $r=0.5$.

[2] M. Kac, Phys. Fluids **2**, 8 (1959).

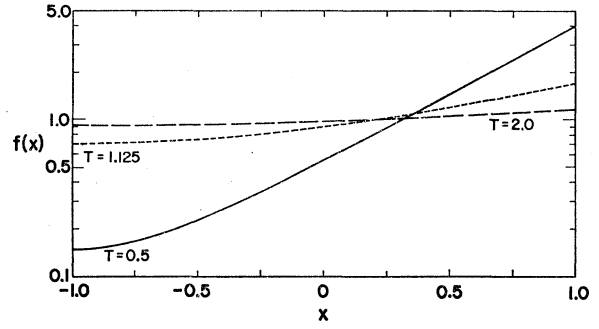

FIG. 2. Probability envelopes for several values of temperature for ferromagnetic type interactions with $r=0.5$.

check on the numerical error in the method previously described. The two methods agreed where the last terms in the power series were neglectable to within about the accuracy prescribed for the termination of the iteration process.

Figures 1–3 illustrate some numerical results for $f(x)$. For $r=0$, it follows immediately from (2.14) that $f(x)=1.0$. For $K=0$ we also have $f(x)=1.0$. As K increases (temperature decreases), $f(x)$ deviates progressively more from a constant. The function, $f(x)$, may be thought of as a probability envelope. That is, there is a set of discrete points (2^N) in $-1\leq x\leq 1$ which have a nonzero probability of occurrence. These probabilities are proportional to $f(x)$. We may therefore compute the expected value of a function, $g(x)$, by iterating (2.11) starting from $f_1(x)=g(x)f(x)$ instead of 1.0. The expected value of $g(x)$ is then,

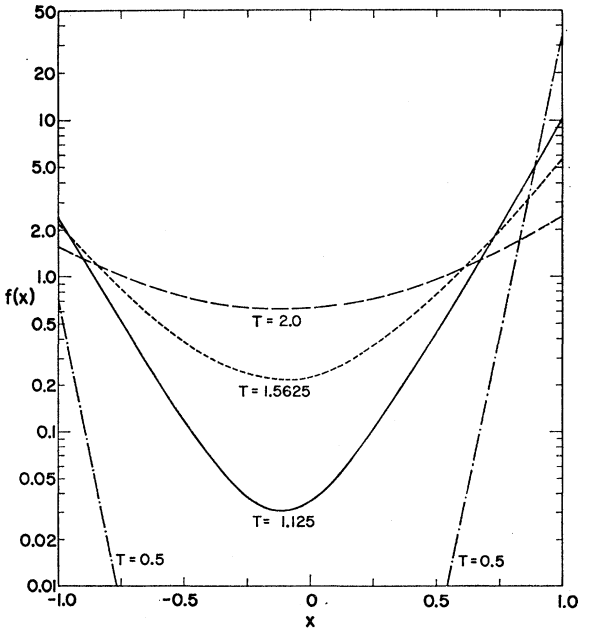

FIG. 3. Probability envelopes for several values of temperature for ferromagnetic type interactions with $r=0.9$.

$$\langle g(x)\rangle=\lim_{M\to\infty}\left(\prod_{j=1}^{M}(\lambda_j/\lambda)\right). \tag{3.9}$$

For example, the energy per particle, is usually given (in appropriate units)

$$E=\partial\ln\lambda(K)/\partial|K|, \tag{3.10}$$

but it may also be computed from (3.9), using

$$g(x)=-Kx/|K|. \tag{3.11}$$

We remark that this procedure has the numerical advantage that one does not have to differentiate to calculate the energy.

Figures 4–6 illustrate the behavior of the energy as

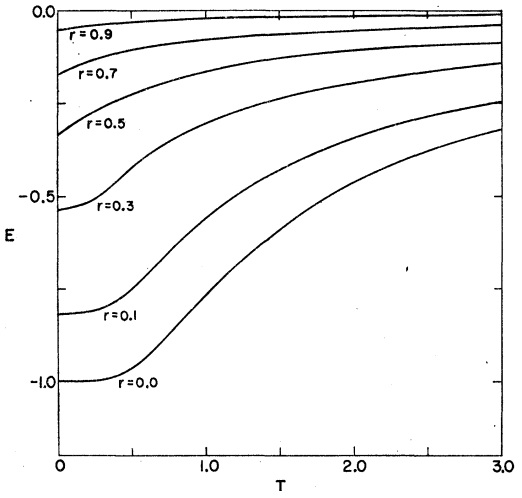

FIG. 4. Energy dependence on temperature for several values of r and antiferromagnetic type interactions.

a function of temperature $(1/|K|)$ for both antiferromagnetic and ferromagnetic type interaction energies. The curves for $r=0$ are, of course, the same for both, and $=-\tanh|K|$.

The value of the energy at zero temperature may be easily obtained by setting

$$g(y)\sim\cosh Ay, \quad |K|\gg 1, \tag{3.12}$$

and solving for A. The result is

$$\begin{aligned} E&=-1.0, && K>0\\ E&=-(1-r)/(1+r), && K<0. \end{aligned} \tag{3.13}$$

The manner in which E tends to zero may be readily obtained from the series expansion. The result is

$$ET\to-(1-r)/(1+r) \tag{3.14}$$

as the temperature, T, tends to infinity.

4. BEHAVIOR NEAR $r=0$

In order to study the behavior of $f(x)$ and $\lambda(K)$ near the short-range limit, $r=0$, it is convenient to recast

Eqs. (3.7) and (3.8) in terms of slightly different variables. If we let

$$d_{\nu,m}=a_{\nu,m}[(1-r)/r^2]^m, \tag{4.1}$$

then (3.7) and (3.8) become

$$\sum_{j=0}^{\nu-\mu} d_{\nu-j,\mu/2}\lambda_j=2\sum_{j=0}^{\mu} r^{\mu-j}(j!)^{-1} \times \sum_{m=[(\mu-j+1)/2]}^{[(\nu-j)/2]} d_{\nu-j,m}\binom{2m}{\mu-j}(1-r)^{m+j-\mu/2}, \tag{4.2}$$

and

$$\lambda_\nu=2\sum_{m=1}^{[\nu/2]} d_{\nu,m}(1-r)^m. \tag{4.3}$$

We may take the limit $r\to 0$ of (4.2) and (4.3) and study the limiting functions so defined, provided that the series so defined converge. We see that only the $j=\mu$ term contributes to the right-hand side of (4.2). Thus, in the limit as $r\to 0$, (4.2) and (4.3) become

$$\sum_{j=0}^{\nu-\mu} d_{\nu-j,\mu/2}\lambda_j=2(\mu!)^{-1}\sum_{m=1}^{[(\nu-\mu)/2]} d_{\nu-\mu,m}, \qquad \lambda_\nu=2\sum_{m=1}^{[\nu/2]} d_{\nu,m}, \tag{4.4}$$

or

$$\sum_{j=0}^{\nu-\mu} d_{\nu-j,\mu/2}\lambda_j=(\lambda_{\nu-\mu})/(\mu!). \tag{4.5}$$

As we pointed out in Sec. 3, the solution of these equations is unique and so we need only exhibit it and verify the solution. It is

$$\begin{aligned} d_{\nu,\mu}&=(\nu!)^{-1}, && \mu=\nu/2\\ &=0, && \mu\neq\nu/2\\ \lambda_\nu&=2(\nu!)^{-1}, && \nu \text{ even}\\ &=0, && \nu \text{ odd}. \end{aligned} \tag{4.6}$$

This result gives the well-known result,

$$\lambda(K)=2\cosh K, \tag{4.7}$$

for λ. The corresponding probability envelope is

$$g(y)=\cosh[ryK/(1-r)^{\frac{1}{2}}], \qquad f(x)=\cosh[rxK/(1-r)^{\frac{1}{2}}+(1-r)^{\frac{1}{2}}K]. \tag{4.8}$$

All these series converge for any value of y or K so that they therefore represent the limiting behavior.

For $r\equiv 0$, Eq. (2.11) may be solved directly. The result is

$$\begin{aligned} f_j(x)&=1.0, && j=1,\cdots,N\\ \lambda_j&=2\cosh K, && j=1,\cdots,N-1. \end{aligned} \tag{4.9}$$

Thus we obtain, for the partition function

$$Z_{N+1}=2(2\cosh K)^{N-1}, \tag{4.10}$$

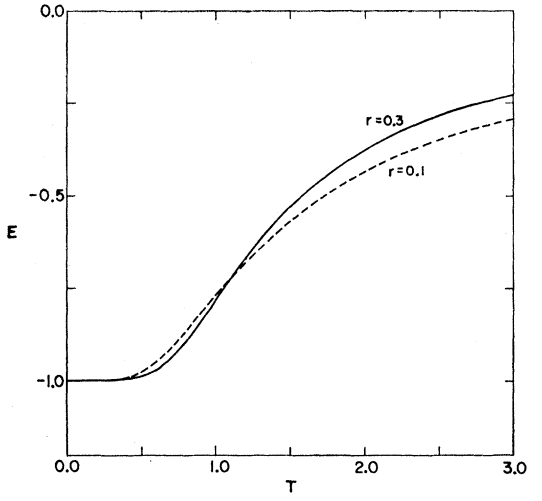

FIG. 5. Energy dependence on temperature for $r=0.1$ and 0.3 for ferromagnetic type interactions.

which is well known to be the correct result when the first and Nth spins are not coupled.

5. BEHAVIOR NEAR $r=1$

We discuss in this section the limiting behavior of the model as $r\to 1$. We must be careful to distinguish, in considering this limit, between the two cases

$$\begin{aligned} &\text{(a)}\quad r\to 1, \quad r^N\to 0;\\ &\text{(b)}\quad r\to 1, \quad r^N\to 1. \end{aligned} \tag{5.1}$$

We will discuss case (a) in this section and we shall discuss case (b) in an Appendix. Case (b) is actually equivalent to the Bragg-Williams approximation. Case (a) is the limit for which the range of the force becomes arbitrarily great, but is still small compared to the total size of the system.

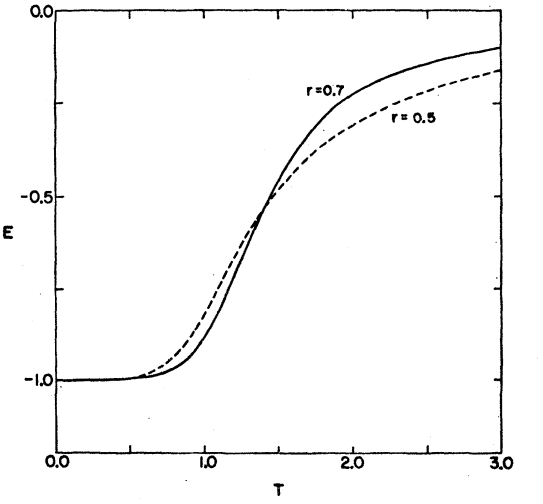

FIG. 6. Energy dependence on temperature for $r=0.5$ and 0.7 for ferromagnetic type interactions.

To discuss case (a), let us first find the limit as $r \to 1$ of the $d_{\nu,m}$ introduced in Sec. 4. Neglecting terms of order $(1-r)^2$ and higher, (4.2) and (4.3) become

$$\sum_{j=0}^{\nu-\mu} d_{\nu-j,\mu/2}\lambda_j \approx 2r^{\mu}[d_{\nu,\mu/2}+\tfrac{1}{2}(\mu+2)(\mu+1)(1-r)d_{\nu,\mu/2+1} +\mu(r^{-1})(1-r)d_{\nu-1,\mu/2}+\tfrac{1}{2}(r^{-2})(1-r)d_{\nu-2,\mu/2-1}] \quad (5.2)$$

$$\lambda_\nu \approx 2d_{\nu,1}(1-r), \quad (5.3)$$

or introducing

$$\Lambda_\nu=\lambda_\nu/(1-r), \quad \nu>0, \quad (5.4)$$

and solving for $d_{\nu,\mu/2}$ we obtain, in the limit as $r \to 1$,

$$d_{\nu,\mu/2}=(\mu+2)(\mu+1)(2\mu)^{-1}d_{\nu,\mu/2+1}+d_{\nu-1,\mu/2} +(2\mu)^{-1}d_{\nu-2,\mu/2-1}-(2\mu)^{-1}\sum_{j=2}^{\nu-\mu} d_{\nu-j,\mu/2}\Lambda_j, \quad (5.5)$$

$$\Lambda_j=2d_{j,1}.$$

If we define

$$d_m(K)=\sum_{\nu=2m}^{\infty} d_{\nu,m}K^\nu, \quad (5.6)$$

we may re-express (5.5) in terms of the $d_m(K)$:

$$[1-K+(2m)^{-1}d_1(K)]d_m(K)=(m+1)(2m+1) \times(2m)^{-1}d_{m+1}(K)+K^2(4m)^{-1}d_{m-1}(K) \quad (5.7)$$

for $m \geq 1$. According to our normalization convention, $d_0(K)=1.0$. Therefore, any $d_1(K)$ determines all the other $d_m(K)$ from (5.7). It follows easily from (5.5) that

$$d_{\nu,m}=0, \quad \nu<2m$$
$$d_{2m,m}=(4^m m!)^{-1}, \quad (5.8)$$
$$d_{2m+1,m}=[4^m(m-1)!]^{-1}.$$

If we now select

$$d_m(K)=(m!)^{-1}\left(\frac{1-(1-2K)^{\frac{1}{2}}}{2}\right)^{2m}, \quad (5.9)$$

we see that

$$d_m(K) \simeq (4^m m!)^{-1}[K^{2m}+mK^{2m+1}+\cdots], \quad (5.10)$$

so that conditions (5.8) are satisfied. [Actually the first of conditions (5.8) is sufficient to determine the $d_m(K)$.] Furthermore, substitution of (5.9) into (5.7) proves that it is satisfied for all $m \geq 1$. Therefore, the unique limiting values of the $d_{\nu,m}$ may be obtained by expanding (5.9) about $K=0$. This result proves that for $|K|<\frac{1}{2}$ [radius of convergence of the power series expansion of the $d_m(K)$],

$$\lim_{r\to 1}\lambda(K)=\lim[2+(1-r)d_1(K)] =2.0. \quad (5.11)$$

Hence the energy, specific heat, etc., tend to zero for $T>2.0$ for both antiferromagnetic and ferromagnetic type interactions.

We note that the $d_m(K)$ may be readily expanded to yield

$$d_{\nu,m}=(\tfrac{1}{2})^{\nu-1}\frac{(2\nu-2m-1)!}{(\nu-2m)!(m-1)!\nu!}. \quad (5.12)$$

We are now in a position to obtain $g(y)$; for, using (5.9) we find in the limit as $r \to 1$

$$g(y) \approx \exp\left(\frac{r^2}{4(1-r)}(1-(1-2K)^{\frac{1}{2}})^2y^2\right), \quad (5.13)$$

and similarly

$$\lambda \approx 2+(1-r)[1-K-(1-2K)^{\frac{1}{2}}]. \quad (5.14)$$

In order to find $g(y)$ when y is not of order $(1-r)^{\frac{1}{2}}$ and $|K|>\frac{1}{2}$, we shall make the substitution

$$g(y)=\exp[G(y)]\cosh[H(y)] \quad (5.15)$$

for $r \neq 1$ where $G(y)$ is an even function and $H(y)$ an odd function. We shall find that $G(y)$ and $H(y)$ are both, in the limit as $r \to 1$, proportional to $(1-r)^{-1}$, and for $K<\frac{1}{2}$, $H(Y) \simeq 0$, in conformity to (5.13). First, if $y \neq 0$, then if

$$q(y)=(1-r)[G'(y)+\tanh H(y)H'(y)], \quad (5.16)$$

we can show by substituting (5.15) into (3.3) and expanding $G(y)$ and $H(y)$ in Taylor series about y that

$$\lambda=2\exp[-yq(y)]\cosh[q(y)+Ky], \quad y\neq 0 \quad (5.17)$$

in the limit as $r \to 1$. On differentiating (5.17) with respect to y, we obtain

$$q'(y)y+q(y)=\tanh[q(y)+Ky] \quad [q'(y)+K]. \quad (5.18)$$

By slightly different manipulations, we can also show that (5.17) and (5.18) hold in the limit as $y \to 0$. The function $q(y)$ is an odd function of y; however, for $y \neq 0$, we see from (5.16) that both even and odd powers of y can appear in its left- and right-hand power series expansion, as $\lim \tanh x$ as $x \to \pm\infty$ is ± 1. We may determine the eigenvalue λ of (5.17) as follows. First, from (5.18),

$$q'(y)=\frac{\{K\tanh[q(y)+Ky]-q(y)\}}{y-\tanh[q(y)+Ky]}. \quad (5.19)$$

If $q(y)$ is to be a solution for all $y \leq 1$, then if the denominator vanishes, the numerator must also, or $q'(y)$ would become infinite. Thus, if

$$y=\tanh[q(y)+Ky], \quad (5.20)$$

then

$$q(y)=K\tanh[q(y)+Ky]. \quad (5.21)$$

As $|\tanh x| \leq 1$, the denominator of (5.19) is clearly greater than or equal to zero for $y=1$. As $q(y) \geq 0$ for all y, there are now two cases to consider. First, the denominator of (5.19) is zero when $y=0$ and second, the denominator of (5.19) is negative when $y=0$. In

the second case, as the denominator of (5.19) changes sign between 0 and 1, there must be a zero for $0<y<1$, and (5.20) and (5.21) must be satisfied at this point to obtain a solution for all y. If we introduce $z=q(y)+Ky$, then at the critical point

$$z=2K\tanh z. \tag{5.22}$$

This equation possesses no real solution other than $z=0$, if $K<\frac{1}{2}$. Thus, we must have $\lambda=2$ for $K<\frac{1}{2}$. It is easy to show that there is a solution of (5.17) for all y for $\lambda=2$ and $K<\frac{1}{2}$. This solution is a direct extension of (5.13) and (5.14). For $K>\frac{1}{2}$, it is easy to find a y (near zero) for which (5.17) has no solution with $\lambda=2$. Thus the first case occurs for and only for $-\infty<K<\frac{1}{2}$. For $K>\frac{1}{2}$ Eq. (5.22) possesses an additional solution besides $z=0$. If z_c is that solution, then

$$\lambda=2\exp[-K\tanh^2 z_c]\cosh[z_c] \tag{5.23}$$

for $K>\frac{1}{2}$. One easily obtains by differentiation of $\ln\lambda$ the following expressions for the energy per spin and the specific heat per spin

$$\begin{aligned} &E=-\tanh^2 z_c, \\ &C_v=[4K^2\tanh^2 z_c\,\mathrm{sech}^2 z_c]/[1-2K\,\mathrm{sech}^2 z_c]. \end{aligned} \tag{5.24}$$

At the critical temperature, $T=2.0$, $z_c=0$, Eq. (5.24) gives

$$\begin{aligned} &E=0,\ C_v=\tfrac{3}{2},\quad T=2.0^-\\ &E=0,\ C_v=0,\quad T=2.0^+. \end{aligned} \tag{5.25}$$

Thus the energy is continuous and the specific heat is discontinuous so that, in the limit as $r\to 1$, this system approaches a second order phase transition.

Figures 7 and 8 illustrate the approach to the limit of $r=1$ for the energy per spin and the specific heat per spin.

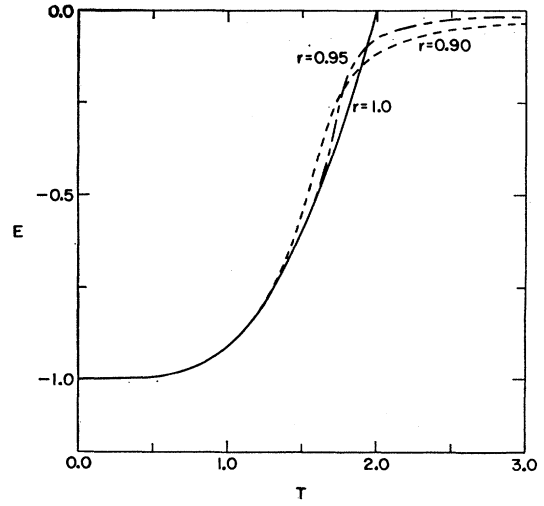

FIG. 7. Approach to the limit, $r=1$, of the energy as a function of temperature for ferromagnetic type interactions.

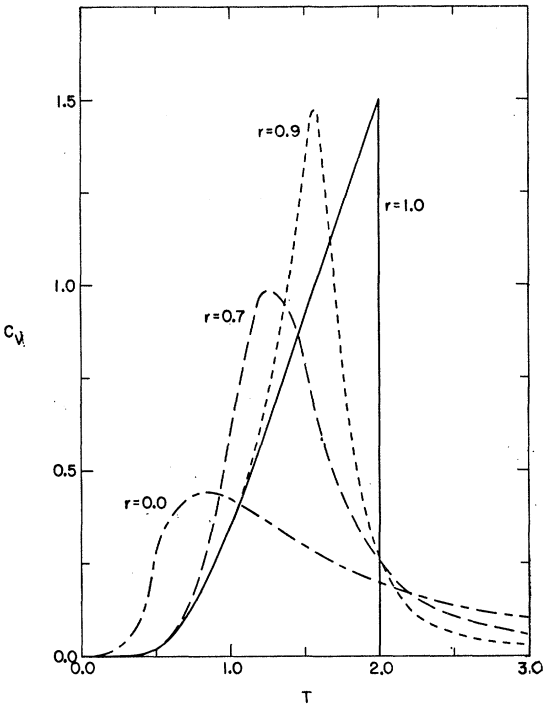

FIG. 8. Approach to the limit, $r=1$, of the specific heat as a function of temperature for ferromagnetic type interactions.

APPENDIX. BRAGG-WILLIAMS LIMIT

In this Appendix we consider case (5.1) (b). The results for this case are well known.[3] We shall, however, give a brief rederivation which illustrates one way that the methods of Kac[2] may be extended. If, instead of (2.8), we define

$$K=Jr(1-r^N)/[(1-r)kT], \tag{A1}$$

then, in the limit (5.1) (b), we may write the total energy of the system as

$$\begin{aligned} E/kT&=-\frac{K}{2N}\Big[\Big(\sum_{j=1}^{N}\nu_j\Big)^2-\sum_{j=1}^{N}\nu_j^2\Big]\\ &=-\frac{K}{2N}\Big(\sum_{j=1}^{N}\nu_j\Big)^2+\tfrac{1}{2}K. \end{aligned} \tag{A2}$$

Suppose we have any system for which the energy is a quadratic form (A is assumed symmetric)

$$\mathcal{E}/kT=-\tfrac{1}{2}\sum_{i,j}\nu_i A_{ij}\nu_j. \tag{A3}$$

If we make use of the well-known integration formula

$$\begin{aligned} \exp\Big\{\tfrac{1}{2}\sum_{i,j}\nu_i A_{ij}\nu_j\Big\}&=(2\pi)^{-N/2}\int_{-\infty}^{+\infty}\cdots\\ &\times\int\exp\Big\{-\tfrac{1}{2}\sum_{i=1}^{N}x_i^2-\sum_{i,j}x_i(A^{\frac{1}{2}})_{ij}\nu_j\Big\}\prod_{j=1}^{N}dx_j, \end{aligned} \tag{A4}$$

[3] See, for instance, D. ter Haar, *Elements of Statistical Mechanics* (Rinehart and Company, New York, 1958), Chap. 12.

we can linearize the exponent in the partition function. Thus

$$Z=(2\pi)^{-N/2}\sum_{\text{all states}}\int_{-\infty}^{+\infty}\cdots$$
$$\times\int\exp\{-\tfrac{1}{2}\sum_{i=1}^{N}x_i^2-\sum_{i,j}x_i(A^{\frac{1}{2}})_{ij}\nu_j\}\prod_{j=1}^{N}dx_j$$
$$=(2\pi)^{-N/2}\int_{-\infty}^{+\infty}\cdots\int\exp\{-\tfrac{1}{2}\sum_{i=1}^{N}x_i^2\}$$
$$\times\mathfrak{M}(x_i)\prod_{j=1}^{N}dx_j \quad \text{(A5)}$$

where $\mathfrak{M}(x_i)$ is defined by

$$\mathfrak{M}(x_i)\equiv\sum_{\text{all states}}\exp\{-\sum_{i,j}x_i(A^{\frac{1}{2}})_{ij}\nu_j\}. \quad \text{(A6)}$$

For certain special cases, $\mathfrak{M}(x_i)$ is particularly simple. The case we are considering is one. The spherical Ising model with interaction energy given by (2.1) is another. If we consider

$$\mathcal{E}=E-\tfrac{1}{2}KkT, \quad \text{(A7)}$$

then

$$A_{ij}=K/N,$$
$$(A^{\frac{1}{2}})_{ij}=K^{\frac{1}{2}}/N,$$
$$\mathfrak{M}(x_i)=\left[\cosh\left\{K^{\frac{1}{2}}\frac{1}{N}\sum_{i=1}^{N}x_i\right\}\right]^N. \quad \text{(A8)}$$

If we make an orthonormal change of variables so that one of the transformed variables is

$$X=\frac{1}{N^{\frac{1}{2}}}\sum_{i=1}^{N}x_i \quad \text{(A9)}$$

and integrate over the others, we obtain

$$Z/2^N=(2\pi)^{-\frac{1}{2}}\int_{-\infty}^{+\infty}\exp(-\tfrac{1}{2}X^2)$$
$$\times\cosh^N[(K/N)^{\frac{1}{2}}X]dX. \quad \text{(A10)}$$

On evaluating (A10) by the method of steepest descents,[4] we obtain the well-known result,

$$\ln\lambda=\lim_{N\to\infty}(\ln Z)/N=\ln 2-\tfrac{1}{2}K\tanh^2 z+\ln\cosh z, \quad \text{(A11)}$$

where, using $z=(K/N)^{\frac{1}{2}}X$, z must satisfy

$$z=K\tanh z. \quad \text{(A12)}$$

For the energy per particle

$$E=-\tfrac{1}{2}\tanh^2 z. \quad \text{(A13)}$$

These results will be seen to be similar, but not identical, to Eqs. (5.22)–(5.24). For corresponding points, the temperature here is half as great and the energy here is also only half as great. The difference between these results and those of Sec. 5 is due, of course, to interchanging the order of the limits $r\to 1$ and $N\to\infty$. The factor of 2 difference in the maximum value of the energy is an obvious consequence of the relative truncation of (A2) compared to (2.1).

The results of this Appendix also indicate that the "high-density limit" in the sense of Brout[5] does not exist. As the ratio of the range of the interaction to the length of the system changes from greater than unity ($1/z=0$) (his 3.2) to zero ($1/z\neq 0$), the maximum interaction energy per spin goes up by a factor of two (in his units). Terms through order $(1-r)$ (that is, $1/z$) in a "high-density" expansion for our model are given by (5.14), for the high-temperature region.

[4] See, for instance, H. Jeffreys and B. S. Jeffreys, *Methods of Mathematical Physics* (Cambridge University Press, New York, 1950), Chap. 17.

[5] R. Brout, Phys. Rev. **118**, 1009 (1960).