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Many-Neighbored Ising Chain

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Using a method suggested by Montroll, we extend the well-known matrix formulation of the nearest-neighbor one-dimensional Ising problem to allow for interactions with an arbitrary finite range n, general spin l, and an applied magnetic field B. We exhibit the relevant matrix element explicitly and hence formally obtain the partition function via an eigenvalue problem of order $(2l+1)^n$. For the case $B=0$, $l=\frac{1}{2}$ we introduce a change of variable which simplifies the partition function while still allowing a matrix formulation. Using this approach we have computed specific-heat curves for infinite, ferromagnetic Ising chains with interactions of range n ($n \leq 7$). We prove in an appendix that open and cyclic boundary conditions are equivalent for the system under consideration.

1. INTRODUCTION

The partition function for an infinite chain of spins was originally calculated by Ising.[1] Kramers and Wannier[2] reformulated the problem in terms of 2×2 matrices. Both of these calculations are restricted to the nearest-neighbor problem. When the interaction is allowed to have an arbitrary finite range, the partition function is harder to calculate; however, Montroll[3] has shown that, in principle, the matrix approach can be applied to this more general problem. Other exact formulations have also been given.[4]

The present paper is devoted in part to an explicit matrix formulation of the many-neighbor problem, based on Montroll's suggestion. The nonsymmetry of the matrices was considered an obstacle by Montroll; this difficulty is removed by a theorem proved in the Appendix.

In Sec. 2 we introduce a change of variable in order to exhibit a relation between the spin-$\frac{1}{2}$ open-chain Ising partition functions for two distinct situations, namely,

(i) no external B field, nearest- and second-nearest-neighbor interactions, and

(ii) external B field applied, nearest-neighbor interactions only.

This relation was first demonstrated by Frankel[5] in another context.

Section 3 deals with the many-neighbored chain of arbitrary spins in an applied B field. We explicitly calculate the general element of a matrix whose largest eigenvalue determines the partition function.

In Sec. 4 we impose the restriction $B=0$, but otherwise retain the generality of Sec. 3. The eigenvalue problem of Sec. 3 is reduced to two eigenvalue problems of lower order.

In Sec. 5 we restrict our attention further to the spin-$\frac{1}{2}$ chain ($l=\frac{1}{2}$) in zero B field. The range (n) of the interaction is still general. We reformulate the problem in terms of the variables described in Sec. 2, and the reduction used in Sec. 4 becomes superfluous.

In Sec. 6 we present computed values of specific heat for the system described in Sec. 5.

In Sec. 7 we discuss other treatments of the one-dimensional Ising problem, particularly those which deal with *infinite*-ranged interactions. We attempt to relate the results of this paper to predictions of critical behavior given by other authors.

Finally, in the Appendix, we prove a theorem to justify a statement made in Sec. 3. The theorem has wider applicability, however, and it amounts to a proof that boundary conditions do not affect the thermodynamic behavior of infinite chains, at least when the interactions have finite range.

2. SIMPLE TREATMENT OF THE CASE $l=\frac{1}{2}$, $B=0$, $n=2$

We consider the spin-$\frac{1}{2}$ chain in zero B field, assuming that spin–spin interactions are negligible except for nearest and second-nearest neighbors. The partition function for a chain of length N is

$$\bar{Q}_N(\beta, J_1, J_2) = \sum_{s_1=-1}^{1} \cdots \sum_{s_N=-1}^{1} \exp \beta \left(J_1 \sum_{i=1}^{N-1} s_i s_{i+1} + J_2 \sum_{i=1}^{N-2} s_i s_{i+2} \right), \quad (2.1)$$

where the coupling constants J_1 and J_2 are positive for a ferromagnetic chain.

[1] E. Ising, Z. Phys. **31**, 253 (1925).

[2] H. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252 (1941). These authors use cyclic boundary conditions leading to an expression for the partition function as the trace of a matrix.

[3] E. W. Montroll, J. Chem. Phys. **10**, 61 (1942). See particularly pp. 68–70.

[4] H. S. Green and J. Liepnik [Rev. Mod. Phys. **32**, 129 (1960)], have developed a "matrix–spinor" approach which has been modified by M. E. Fisher and H. N. V. Temperley, Rev. Mod. Phys. **32**, 1029 (1960). The recursion relations they obtain may well be suited to an exact numerical treatment of the many-neighbored Ising chain.

[5] N. E. Frankel and D. Rapaport (to be published).

We define a new set of variables $\{t_i\}$ with possible values ± 1:

$$t_0 = s_1$$
$$t_i = s_i s_{i+1}, \quad i = 1, 2, \cdots, N-1. \tag{2.2}$$

In the spin-$\frac{1}{2}$ case this transformation can be uniquely inverted since $s_i^2 \equiv 1$ so that

$$s_i = s_i s_{i-1} s_{i-1} s_{i-2} s_{i-2} \cdots s_2 s_1 s_1 = t_{i-1} t_{i-2} \cdots t_1 t_0. \tag{2.3}$$

Thus for each set of values $\{s_i\}$ there is exactly one set $\{t_i\}$ and vice versa. Hence the partition function becomes

$$\bar{Q}_N(\beta, J_1, J_2) = 2 \sum_{t_1=-1}^{1} \cdots \sum_{t_{N-1}=-1}^{1} \exp \beta \left(J_1 \sum_{i=1}^{N-1} t_i + J_2 \sum_{i=1}^{N-2} t_i t_{i+1} \right), \tag{2.4}$$

where $s_i s_{i+2} = s_i (s_{i+1})^2 s_{i+2} = t_i t_{i+1}$, and the factor 2 arises from the sum over t_0.

Now the partition function for the spin-$\frac{1}{2}$ nearest-neighbor chain in a magnetic field B is given by

$$Q_N(\beta, J, B) = \sum_{s_1=-1}^{1} \cdots \sum_{s_N=-1}^{1} \exp \beta \left(\mu B \sum_{i=1}^{N} s_i + J \sum_{i=1}^{N-1} s_i s_{i+1} \right). \tag{2.5}$$

Hence, from comparison of (2.4) and (2.5),

$$\bar{Q}_N(\beta, J_1, J_2) = 2 Q_{N-1}(\beta, J, B), \tag{2.6}$$

where $J = J_2$ and $\mu B = J_1$.

Thus the second-nearest-neighbor result can be transcribed from the well-known nearest-neighbor result.[6] The relation (2.6) was first noticed by Frankel[5] in another context.

The transformation (2.2) can only be used in the spin-$\frac{1}{2}$ case for which the unique inverse (2.3) exists; a further restriction is that the applied field B is zero. However the technique is *not* restricted to the second-nearest-neighbor problem and we use (2.2) in Sec. 5 in the context of long-ranged interactions.

3. GENERAL PARTITION FUNCTION

We consider the case of general spin with an external magnetic field B.

Let each site have spin l so that the spin projection s_i can take $2l + 1$ values.

We consider an n-neighbor chain; thus the interaction energy of two spins is

$$E(s_i, s_{i\pm k}) = \begin{cases} -J_k s_i s_{i\pm k}, & \text{when } 0 < k \leq n, \\ 0, & \text{when } k > n. \end{cases}$$

In order to write down the energy of the chain in any given configuration we divide the chain into blocks of length n and consider a chain of total length Nn. This procedure was suggested by Montroll[3] who performed the calculation explicitly for the case $l = \frac{1}{2}$, $n = 2$, $B = 0$.

The division is as follows:

1st block	2nd block	$\cdots$	jth block	$\cdots$	Nth block
$[s_1 \; s_2 \; \cdots \; s_n]$	$[s_{n+1} \; s_{n+2} \; \cdots \; s_{2n}]$	$\cdots$	$[s_{(j-1)n+1} \; \cdots \; s_{jn}]$	$\cdots$	$[s_{(N-1)n+1} \; \cdots \; s_{Nn}]$
or $[s_1^{(1)} \; \cdots \; s_n^{(1)}]$	$[s_1^{(2)} \; \cdots \; s_n^{(2)}]$	$\cdots$	$[s_1^{(j)} \; \cdots \; s_n^{(j)}]$	$\cdots$	$[s_1^{(N)} \; \cdots \; s_n^{(N)}]$,

where the second alternative is merely a convenient relabeling of the first.

Each block has $(2l + 1)^n$ possible configurations, so that the configuration of the jth block can be specified by a single integer c_j where $1 \leq c_j \leq (2l + 1)^n$. Because the interaction has range n, a spin in the jth block can interact only with spins in the $(j-1)$th, jth, and $(j+1)$th blocks. Hence the energy of the chain is the sum of three types of term:

(i) interaction energies with the external B field,

(ii) mutual energies of spins which are in the same block, and

(iii) mutual energies of spins from two adjacent blocks.

The contributions of types (i) and (ii) from the jth block are

$$X_{c_j} \equiv X(s_1^{(j)}, s_2^{(j)}, \cdots, s_n^{(j)}) = -\mu B \sum_{i=1}^{n} s_i^{(j)} - \sum_{k=1}^{n} J_k \left(\sum_{i=1}^{n-k} s_i^{(j)} s_{i+k}^{(j)} \right). \tag{3.1}$$

The contribution of type (iii) from the jth and $(j+1)$th blocks is

$$Y_{c_j, c_{j+1}} \equiv Y(s_1^{(j)}, \cdots, s_n^{(j)}; s_1^{(j+1)}, \cdots, s_n^{(j+1)}) = -\sum_{k=1}^{n} J_k \left(\sum_{i=1}^{k} s_{n+1-i}^{(j)} s_{k-i+1}^{(j+1)} \right). \tag{3.2}$$

Note that if the configurations of blocks j and $(j+1)$ are interchanged their mutual energy is *not* invariant; that is, the matrix Y is nonsymmetric.

The total energy of the chain in configuration $(c_1, c_2, \cdots, c_N)$ is

$$H(c_1, \cdots, c_N) = X_{c_1} + Y_{c_1, c_2} + X_{c_2} + Y_{c_2, c_3} + \cdots + Y_{c_{N-1}, c_N} + X_{c_N}.$$

[6] The simplest derivation of the nearest-neighbor result (that of Ref. 2) uses cyclic boundary conditions whereas we use open-chain conditions to derive (2.6). However the appendix to this paper is a rigorous proof that the boundary conditions are unimportant. See also the remarks at the end of Sec. 3.

Defining a matrix V and a vector $\mathbf{U}$ by the relations

$$V_{c_i,c_j} = \exp -\beta(\tfrac{1}{2}X_{c_i} + Y_{c_i,c_j} + \tfrac{1}{2}X_{c_j}),$$
$$U_{c_i} = \exp -\tfrac{1}{2}\beta X_{c_i}, \tag{3.3}$$

we find that the partition function is

$$\begin{aligned} Q_{Nn} &= \sum_{c_1}\cdots\sum_{c_N} \exp -\beta H(c_1,\cdots,c_N) \\ &= \sum_{c_1}\cdots\sum_{c_N} U_{c_1}V_{c_1,c_2}V_{c_2,c_3}\cdots V_{c_{N-1},c_N}U_{c_N} \\ &= \mathbf{U}^{\mathrm{T}}V^{N-1}\mathbf{U} \end{aligned} \tag{3.4}$$

The vector $\mathbf{U}$ can be regarded as representing end effects due to a deficiency of neighbors for the spins near the ends of the chain.

Because V is, in general, nonsymmetric, it may not be similar to any diagonal matrix and the rigorous evaluation of (3.4) is not quite straightforward, even in the limit $N \to \infty$. For example, Montroll, in calculating the second-nearest-neighbor partition function from a formula similar to (3.4), was obliged to exhibit a full orthonormal set of left and right eigenvectors for his matrix; the existence of such a set is not automatic for a nonsymmetric matrix.

We overcome this difficulty in a completely general fashion in the Appendix, where we show that the Q_{Nn} of Eq. (3.4) has the following property:

$$(\log Q_{Nn})/(N-1) \to \log \lambda_1, \quad \text{as} \quad N \to \infty, \tag{3.5}$$

where λ_1 is the positive, nondegenerate, largest eigenvalue of V. The *only* conditions necessary for this result are that V and $\mathbf{U}$ are of finite size and have positive elements.

If we had applied cyclic boundary conditions[2] to the chain, the formula (3.4) would have been

$$Q_{Nn} = \mathrm{Tr}\, V^N.$$

Now it is easily proved that, for *any* $M \times M$ matrix V,

$$\mathrm{Tr}\, V^N = \sum_{i=1}^{M} \lambda_i^N,$$

where λ_i are the M (possibly degenerate) eigenvalues of V. Hence, for cyclic boundary conditions

$$Q_{Nn} \sim \lambda_1^N,$$

where λ_1 is the dominant eigenvalue of V.

Therefore, the appendix is actually a rigorous demonstration that open and cyclic boundary conditions lead to the same thermodynamic behavior for the type of system we have been considering.

4. REDUCTION OF THE GENERAL EIGENVALUE PROBLEM[7]

When there is no external B field the energy of the chain is unaltered by a complete "spin flip"; in fact the matrix V of (3.3) has the following property:

$$\begin{aligned} &V(s_1,\cdots,s_N;s_1',\cdots,s_N') \\ &\quad = V(-s_1,\cdots,-s_N;-s_1',\cdots,-s_N'), \\ &\qquad \text{for} \quad B = 0. \end{aligned} \tag{4.1}$$

Also, if the spin l is an integer, s_i may take the value zero and clearly

$$V(0,\cdots,0;s_1,\cdots,s_N) = V(s_1,\cdots,s_N;0,\cdots,0). \tag{4.2}$$

From (4.1) and (4.2) it follows that, by suitably ordering the configurations c_j, we can cast V into the following partitioned form:

$$V = \left(\begin{array}{c|c} A & B \\ \hline B & A \end{array}\right), \quad \text{for half-integral } l,$$

or

$$V = \left(\begin{array}{c|c|c} C & \mathbf{x} & D \\ \hline \mathbf{x}^{\mathrm{T}} & 1 & \mathbf{x}^{\mathrm{T}} \\ \hline D & \mathbf{x} & C \end{array}\right), \quad \text{for integral } l.$$

Here A, B, C, and D are square matrices whose dimension is the greatest integer l' not exceeding $(2l+1)^n/2$. $\mathbf{x}$ is a column vector of dimension l'.

Defining the orthogonal matrices

$$T_1 = 2^{-\frac{1}{2}}\left(\begin{array}{c|c} I & I \\ \hline I & -I \end{array}\right) = T_1^{-1},$$

$$T_2 = 2^{-\frac{1}{2}}\left(\begin{array}{c|c|c} I & \mathbf{O} & I \\ \hline \mathbf{O}^{\mathrm{T}} & 2^{\frac{1}{2}} & \mathbf{O}^{\mathrm{T}} \\ \hline I & \mathbf{O} & -I \end{array}\right) = T_2^{-1},$$

we find that

$$T_1 V T_1^{-1} = \left(\begin{array}{c|c} A+B & 0 \\ \hline 0 & A-B \end{array}\right), \quad \text{for half-integral } l,$$

$$T_2 V T_2^{-1} = \left(\begin{array}{c|c|c} C+D & 2^{\frac{1}{2}}\mathbf{x} & 0 \\ \hline 2^{\frac{1}{2}}\mathbf{x}^{\mathrm{T}} & 1 & \mathbf{O}^{\mathrm{T}} \\ \hline 0 & \mathbf{O} & C-D \end{array}\right), \quad \text{for integral } l. \tag{4.3}$$

Equation (4.3) shows that the dominant eigenvalue of V is equal to the dominant eigenvalue of one of two smaller matrices, each of approximately one-half the

[7] This paragraph generalizes the work of Montroll (Ref. 3) and includes as a special case the reduction of M. Suzuki, B. Tsujiyama, and S. Katsura, J. Math. Phys. **8**, 124 (1967).

dimension of V. With reference to the right-hand side of (4.3), we believe that it is always the *upper* submatrix which contributes the dominant eigenvalue of V, but we have not proved this.

5. REDUCTION OF EIGENPROBLEM FOR SPIN $\frac{1}{2}$

In the case $B = 0$, $l = \frac{1}{2}$, the entire problem may be reformulated in terms of the variables t_i defined by (2.2). The result is a *single* eigenproblem of order 2^{n-1} instead of *two* such problems as in Sec. 4.

For an interaction of range n we consider a chain of length $N(n-1)+1$. When $B = 0$, the energy of the chain is independent of t_0:

$$\begin{aligned} H(t_1, \cdots, t_{Nm}) &= -J_1\{t_1 + t_2 + \cdots + t_{Nm}\} \\ &\quad - J_2\{t_1t_2 + \cdots + t_{Nm-1}t_{Nm}\} - \cdots \\ &\quad - J_n\{t_1t_2\cdots t_m + \cdots + t_{m(N-1)+1}\cdots t_{Nm}\}, \end{aligned} \tag{5.1}$$

where we have temporarily put $(n-1) \equiv m$.

Again we impose a grouping of the variables into blocks:

$$[t_1^{(1)}, \cdots, t_{n-1}^{(1)}]\,[t_1^{(2)}, \cdots, t_{n-1}^{(2)}]\cdots[t_1^{(N)}, \cdots, t_{n-1}^{(N)}].$$

The products $t_it_{i+1}\cdots t_{i+k}$ occurring in (5.1) are of two types:

(i) t_i and t_{i+k} may be in the same block,
(ii) t_i and t_{i+k} may be in adjacent blocks.

The contribution of type (i) from the jth block is

$$\begin{aligned} \bar{X}_{c_j} &\equiv \bar{X}(t_1^{(j)}, \cdots, t_{n-1}^{(j)}) \\ &= -\sum_{k=1}^{n-1} J_k \sum_{i=1}^{n-k} t_i^{(j)} t_{i+1}^{(j)} \cdots t_{i+k-1}^{(j)} \end{aligned} \tag{5.2}$$

and the contribution of type (ii) from blocks j and $(j+1)$ is

$$\begin{aligned} \bar{Y}_{c_j,c_{j+1}} &\equiv \bar{Y}(t_1^{(j)}, \cdots, t_{n-1}^{(j)}; t_1^{(j+1)}, \cdots, t_{n-1}^{(j+1)}) \\ &= -\sum_{k=2}^{n} J_k \sum_{i=1}^{k-1} t_{n-i}^{(j)} t_{n-i+1}^{(j)} \cdots t_{n-1}^{(j)} t_1^{(j+1)} \cdots t_{k-i}^{(j+1)}. \end{aligned} \tag{5.3}$$

As in Sec. 3, we define

$$\begin{aligned} \bar{V}_{c_j,c_{j+1}} &= \exp -\beta(\tfrac{1}{2}\bar{X}_{c_j} + \bar{Y}_{c_j,c_{j+1}} + \tfrac{1}{2}\bar{X}_{c_{j+1}}), \\ \bar{U}_{c_j} &= \exp -\tfrac{1}{2}\beta\bar{X}_{c_j}, \end{aligned} \tag{5.4}$$

and once more the partition function has the form

$$\bar{Q}_{Nm+1} = 2\bar{\mathbf{U}}^{\mathrm{T}}\bar{V}^{N-1}\bar{\mathbf{U}}, \quad 2 \equiv \sum_{t_0=-1}^{1}, \tag{5.5}$$

where the dimension of $\bar{\mathbf{U}}$ and $\bar{V}$ is 2^{n-1} and both have positive elements. The result of the Appendix is again applicable:

$$(\log \bar{Q}_{Nm+1})/N - 1 \to \log \lambda_{\max}, \quad \text{as} \quad N \to \infty,$$

where $\lambda_{\max}$ is the dominant eigenvalue of $\bar{V}$.

6. NUMERICAL RESULTS

Using the matrix defined by Eqs. (5.2)–(5.4), we have programmed a digital computer to calculate specific heat curves for the spin-$\frac{1}{2}$ chain in zero B-field. Considerations of computer time and storage space limited the treatment to cases where the interactions have range less than 8 lattice spacings: even so, 64×64 matrices were processed.

In order to test a conjecture made by Kac (see Sec. 7), we chose the mutual energy of two spins to be

$$E_{ij} = \begin{cases} -Js_is_j/|i-j|^p, & |i-j| \le n, \\ 0, & |i-j| > n, \end{cases}$$

where n is the range of the interaction.

The specific-heat curves are shown in Figs. (1)–(4) for various values of n and p.

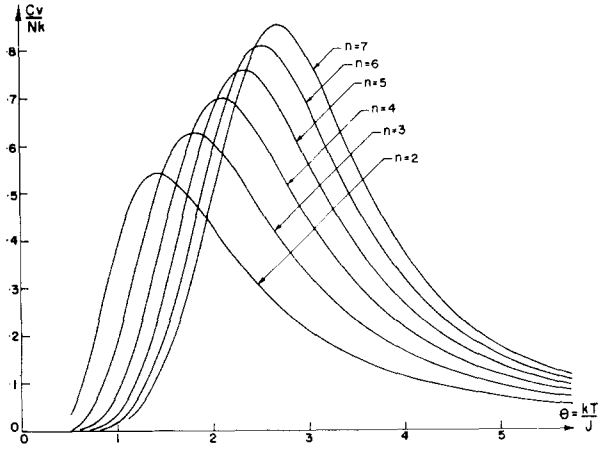

FIG. 1. $p = 1.2$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{1.2}, \quad |i-j| \le n.$$

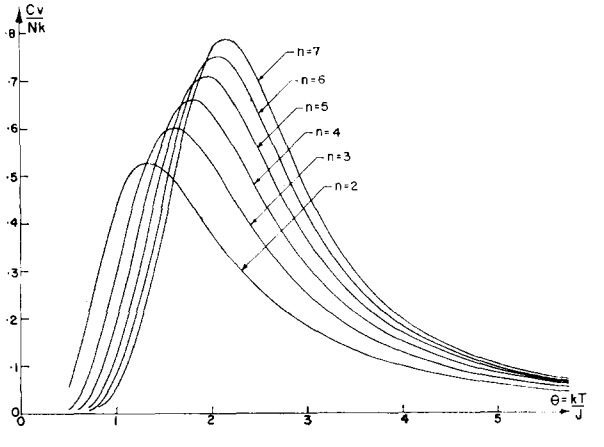

FIG. 2. $p = 1.5$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{1.5}, \quad |i-j| \le n.$$

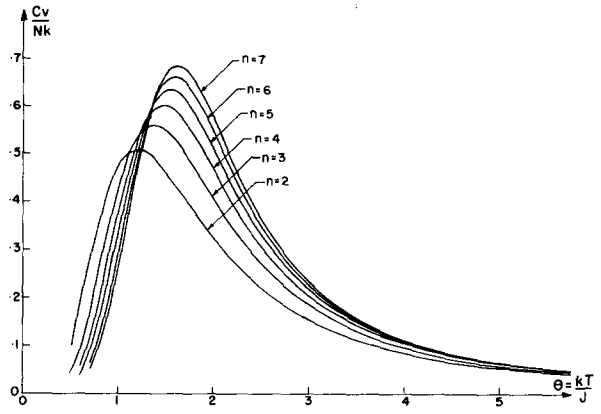

FIG. 3. $p = 2.0$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{2.0}, \quad |i-j| \leq n.$$

A direct method has been used elsewhere to calculate the partition function and specific heat for *finite* chains of length 6 and 7 with all spins interacting.[8] The results of the direct calculation do not differ greatly from those shown in Figs. (1)–(4). The infinite chain considered here naturally gives rise to slightly more sharply peaked curves, while the maxima occur at somewhat higher temperatures.

7. DISCUSSION

The one- and two-dimensional Ising models differ fundamentally in that no phase transition occurs in one dimension for any finite-ranged interaction,[9] while in two dimensions even a nearest-neighbor interaction results in a phase transition.[10] However it is known that in both one and two dimensions a potential of the form

$$H(s_1, \cdots, s_N) = -(J/N) \sum_{1 \leq i < j \leq N} s_i s_j, \quad N \to \infty,$$

leads to a finite discontinuity in the specific heat (the well-known "molecular field theory" type of phase transition). Domb[11] and Kac[12] have raised the question of phase transitions for a more physical infinite-ranged potential of the form

$$E_{ij} = -Js_i s_j/|i-j|^p.$$

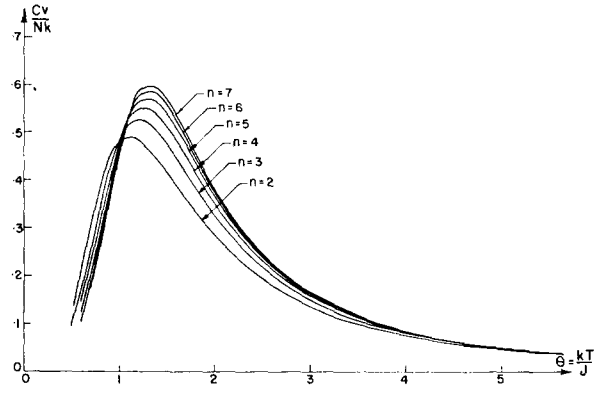

FIG. 4. $p = 2.5$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{2.5}, \quad |i-j| \leq n.$$

Kac conjectures that in one dimension a phase transition does occur when $1 < p \leq 2$, but not when $p > 2$.

Unfortunately the potentials treated in Sec. 6 do not have a long enough range to test Kac's conjecture conclusively. However for the case $p = 2.5$ [Fig. (4)] it seems clear that as the range (n) of the interaction increases the specific-heat plots are converging to a smooth curve with no discontinuity or divergence. For p between 1 and 2 the results are not inconsistent with a molecular-field type of transition but other kinds of behavior cannot be ruled out.

The curves do, however, permit an estimate to be made of the Curie temperature for an infinite-ranged potential (more strictly, a lower bound can be given for $\theta_{\max}$, the temperature at which the specific heat has its maximum value, finite or infinite; see Table I). The result quoted in Table I for $p = 2.0$ is

TABLE I. Estimates of the "Curie" temperature for an infinite-ranged interaction $1/r^p$.

p	$\theta_{\max}$
1.0	>3.1 (unphysical)
1.2	>2.7
1.5	>2.1
1.8	$\gtrsim 1.85$
2.0	$\gtrsim 1.63$
2.2	$\gtrsim 1.47$

in good agreement with a calculation by Joyce[13] who used series expansions to investigate the zero-field magnetic susceptibility of a chain with an infinite-ranged potential $J/|i-j|^2$. He obtained a Curie temperature of $\theta_c = 1.6_8$, compared with $\theta_{\max} \gtrsim 1.6_3$ as shown above.

[8] D. Rapaport (private communication).

[9] E. W. Montroll, J. Chem. Phys. **9**, 706 (1941). In particular, see p. 711. Montroll notes that the dominant eigenvalue of the matrix V must become degenerate if a phase transition is to occur. The theorem of Ref. 14 (see also the Appendix) rules out this degeneracy for a finite-ranged interaction.

[10] The first solution of the two-dimensional problem was given by L. Onsager, Phys. Rev. **65**, 117 (1944).

[11] C. Domb, in *Critical Phenomena, Proceedings of a Conference, Washington, D.C., 1965* (U.S. National Bureau of Standards, Washington, D.C., 1966); N.B.S. Misc. Publ. 273.

[12] M. Kac, *Brandeis Summer School Lectures, 1966* (to be published).

[13] G. S. Joyce, quoted by C. Domb (see Ref. 11, particularly p. 39).

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APPENDIX

Let

$$Q_N = \mathbf{U}^{\mathrm{T}} V^N \mathbf{W} = \sum_{s=1}^{R} \sum_{s'=1}^{R} U_s (V^N)_{ss'} W_{s'}, \tag{A1}$$

where V is an $R \times R$ matrix with positive elements, and $\mathbf{U}$ and $\mathbf{W}$ are column vectors with positive elements.

Then (i) V has a nondegenerate eigenvalue λ_1 of largest modulus and $\lambda_1 > 0$ (this follows from a theorem of Frobenius[14]) and (ii) there exists a *positive* constant C such that

$$Q_N/\lambda_1^N \to C \quad \text{as} \quad N \to \infty.$$

(Since we are to take logarithms of this relation it is essential that $C \neq 0$.)

Proof of (ii)*:* Any matrix V can be factorized in *Jordan canonical form*

$$V = P\Delta P^{-1}, \qquad V^N = P\Delta^N P^{-1}, \tag{A2}$$

where P is nonsingular and Δ is the direct sum of simple Jordan matrices D_i:

$$\Delta = \operatorname{diag}(D_1, D_2, \cdots, D_M).$$

Corresponding to each *nondegenerate* eigenvalue λ the simple Jordan matrix is just the 1×1 matrix λ. However, to each *degenerate* eigenvalue λ_i there correspond one or more matrices D_i of the form

$$(D_i)_{\alpha\beta} = \lambda_i \delta_{\alpha\beta} + \delta_{\alpha+1,\beta}. \tag{A3}$$

(For matrices with complete eigenvector spaces the D_i are all 1×1 but for less well-behaved matrices the D_i are larger.)

We order the eigenvalues of V according to their modulus, $\lambda_1 > |\lambda_2| \geq |\lambda_3| \cdots \geq |\lambda_R|$. Since λ_1 is nondegenerate, D_1 is 1×1 and

$$\Delta = \operatorname{diag}(\lambda_1, D_2, \cdots, D_M)$$

so that

$$\Delta^N/\lambda_1^N = \operatorname{diag}(1, D_2^N/\lambda_1^N, \cdots, D_M^N/\lambda_1^N). \tag{A4}$$

[The basic aim is to show that all terms on the rhs of (A4) approach zero, except for the first term.]

From (A3) it follows by induction (or merely by inspection) that

$$(D_i^N)_{\alpha\beta} = \sum_{r=0}^{M_i - 1} \lambda_i^{N-r}\, {}^N C_r \delta_{\alpha+r,\beta}$$

where D_i is $M_i \times M_i$, i.e.,

$$(D_i^N)_{\alpha\beta} = \begin{cases} 0, & (\beta - \alpha) > N, \\ \lambda_i^{N-\beta+\alpha}\, {}^N C_{\beta-\alpha}, & N \geq (\beta - \alpha) \geq 0, \\ 0, & (\beta - \alpha) < 0. \end{cases}$$

Further routine manipulation shows that, for $N > 2\delta \equiv 2\,|\beta - \alpha|$,

$$|(D_i^N)_{\alpha\beta}/\lambda_1^N| \leq [\lambda_1^{\delta}\, |\lambda_2/\lambda_1|^{N/2-\delta}\, N^{\delta}]\, |\lambda_2/\lambda_1|^{N/2}, \quad \text{for} \quad i \geq 2,$$

where the term in square brackets is bounded (and in fact it $\to 0$) as $N \to \infty$.

Thus, for $i > 1$,

$$(D_i^N)_{\alpha\beta}/\lambda_1^N = O(p^N), \quad \text{as} \quad N \to \infty, \tag{A5}$$

where

$$p = |\lambda_2/\lambda_1|^{\frac{1}{2}} < 1.$$

(A4) and (A5) lead to the result

$$(\Delta^N)_{\alpha\beta}/\lambda_1^N = \delta_{\alpha 1}\delta_{1\beta} + O(p^N). \tag{A6}$$

This is the required "smallness condition" mentioned after Eq. (A4).

Substituting (A6) into (A2) we obtain

$$(V^N)_{\alpha\beta}/\lambda_1^N = P_{\alpha 1}(P^{-1})_{1\beta} + O(p^N), \tag{A7}$$

since a constant, finite, linear combination of $O(p^N)$ quantities is rigorously $O(p^N)$.

Now (A7) shows that

$$P_{\alpha 1}(P^{-1})_{1\beta} \geq 0; \tag{A8}$$

for V has positive elements and $\lambda_1 > 0$ so that $(V^N)_{\alpha\beta}/\lambda_1^N > 0$ for all finite N.

Combining (A1) and (A7),

$$Q_N/\lambda_1^N = \left[\sum_{\alpha,\beta} U_\alpha P_{\alpha 1}(P^{-1})_{1\beta} W_\beta\right] + O(p^N). \tag{A9}$$

Now the quantities $(P)_{\alpha 1}(P^{-1})_{1\beta}$ are nonnegative [by Eq. (A8)] and they cannot be zero for all α, β since this would make either P of P^{-1} singular, contrary to (A2). Hence from the positiveness of U_α and W_β, the quantity in square brackets in (A9) is positive, i.e.,

$$Q_N/\lambda_1^N \to C, \quad \text{as} \quad N \to \infty, \tag{A10}$$

where

$$C = \left[\sum_{\alpha,\beta} U_\alpha P_{\alpha 1}(P^{-1})_{1\beta} W_\beta\right] > 0. \qquad \text{Q.E.D.}$$

Taking logarithms of (A10) we find that

$$(\log Q_N)/N \to \log \lambda_1 \quad \text{as} \quad N \to \infty.$$

[14] S. B. Frobenius, Preuss. Akad. Wiss. 514 (1909).