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Cell Model of a Fluid. I. Evaluation of the Partition Function and Series Expansions

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The partition function of a one-dimensional system of particles with all interactions active is formulated in terms of Ising ferromagnetic spin states. It is shown how the partition function for two- and three-dimensional systems can be obtained from the one-dimensional one by restricting the number of bonds per particle. After writing the partition function in matrix form, the operator of interest is diagonalized and its trace expressed in the form of a convenient infinite series. The series is shown to be absolutely convergent and its analytic properties are briefly investigated. It is then applied to one-, two-, and three-dimensional systems with nearest-neighbor interactions. The validity of the model is established by summing the one-dimensional series and comparing it with the known solution obtainable by other methods. Two- and three-dimensional series are determined by algebraic techniques identical to the one-dimensional series. These are seen to agree with the low-temperature expansions obtained by other authors. The method of this article is seen to have the advantage of simplicity and uniformity regardless of the dimension of the system. A subsequent article is devoted to the thermodynamics of the model.

1. INTRODUCTION

It is well known that it has not been possible as yet to formulate a completely satisfactory molecular theory of the liquid state which correctly portrays phase transitions and remains valid in the transition region. Basically, the difficulty lies in the high densities of liquids which approach those of solids, while symmetries of the solid state are lacking. Consequently, in liquid theory one is forced to deal with a general N-body problem without recourse to the simplifications and approximations that are available in dealing with solids and gases. Nor has it proved feasible thus far to extend the cluster expansions and virial series to the transition region itself and to liquids.[1–4] While these series converge absolutely and generally quite rapidly for gases, it has not been possible to extend these analytically to other phase regions. In view of the work of Yang and Lee, such an extension may well be impossible on theoretical grounds,[5] since, in the thermodynamic limit, it seems probable that the logarithm of the partition function is a lacunary function[6] with a solid wall of singularities surrounding the origin in the complex y plane (y = activity). Not surprisingly, there have been very few successful attempts to find an exact mathematical representation of a system exhibiting a phase transition. Some typical exceptions are the two-dimensional Ising model,[7,8] the ideal Bose gas,[3] the spherical Ising model,[9,10] and the Kac–Baker model.[4,11–13] All but two of these deal with models in one and two dimensions. While these do not correspond to any real system except perhaps a surface film or filament, they have the decisive advantage of being mathematically tractable. One hopes, then, that some of the conclusions and properties of these models may generalize to three dimensions.

We address ourselves in this series of two articles to the study of a simple one-dimensional model. Van Hove has shown that one-dimensional systems with finite-range pairwise potentials with a cutoff will show no phase transition.[14] Accordingly, the interaction potential chosen for the model investigated here has an infinite range with a hard-rod repulsive core and possesses, as we shall see, variable range and depth parameters. In these respects the model resembles the Kac–Baker one, but it differs from the latter in the analysis and technique of solution. Moreover, the potential is a modified Lennard–Jones one, rather than the exponential interaction potential used by Kac and Baker. The system investigated here is a cell model of a simple fluid in which the cells have

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the purpose of specifying the instantaneous location of the particles with an uncertainty equal to the cell parameter. It is therefore not a lattice gas in the usual sense, since the particles are not fixed at their lattice sites but are free to move throughout the system. We shall find that, by selecting the cell parameter equal to the particle's exclusion length, we are able to separate completely the repulsive-core potential from the attractive tail. This choice is equivalent to introducing an exclusion principle into the system which limits cell occupancy to one particle or none. It is therefore convenient to designate such occupancy by means of Ising spin indices. We shall see, however, that the spinor-algebraic approach which proved so successful in the two-dimensional Ising model appears not to lead to a solution in the present instance. This is because the infinite-range potential causes every particle to interact with every other one, so that in the thermodynamic limit the coordination number becomes infinite. It is possible, however, to linearize the partition function by a Fourier-type transform, thereby obtaining a solution of the problem in the form of an infinite series which converges absolutely for all finite values of the activity. By applying the solution to a nearest-neighbor potential, one can confirm the validity of the approach, since the series can then be summed and compared with the known closed-form solution. This calculation at the same time lays the ground work for obtaining low-temperature series in two and three dimensions by identical algebraic techniques. We shall prove that, in order to obtain such series, one need only modify the interaction potential in a suitable way. It will be established that by this simple stratagem two- and three-dimensional systems with more limited interactions can be generated from the basic one-dimensional model. While it is not necessary to restrict the interaction to nearest neighbors in these higher-dimensional systems, it is essential that the coordination number remain small so that the approach be mathematically tractable. The resulting series will be seen to agree completely with those obtained by other authors.

The thermodynamics of this model will be explored in the second article of this series. We shall find there that the behavior is surprisingly realistic and that the system undergoes a change of phase under certain conditions.

2. MATHEMATICAL FORMULATION OF THE PROBLEM

A. One-Dimensional System

The basic system considered is a one-dimensional fluid in which every particle interacts with every other one. Extension to higher dimensions will be considered later. Let the particles be distributed on a line of length L, bent to form a ring. All distance measurements then occur mod. N. The periodic boundary condition is introduced for mathematical convenience only; it becomes insignificant in the thermodynamic limit. We divide the line into N equal segments or cells, each of length $l = L/N$. Cells may be either occupied or empty, particles being free to move from one cell to the next. The particles are assumed to be completely symmetric and to interact with a modified Lennard–Jones potential of the form

$$V(x) = \begin{cases} +\infty & (x < l/2), \\ -\zeta/|x|^{\gamma} & (x \geq l/2), \end{cases} \tag{2.1}$$

where x is the separation between particles, ζ is the potential depth, and γ is a parameter fixing the range of interaction. The hard-core repulsive interaction is most conveniently accounted for by letting the cell-size l coincide with the exclusion length of the particle and restricting cell occupation numbers to zero and one. All other choices of l can be shown to be trivial variations of this scheme. The interaction potential in terms of the present discrete model is then

$$\phi_s = \tfrac{1}{2}(V_s + V_{N-s}),$$
$$V_s = \begin{cases} 0 & (s = 0) \\ -\zeta/s^{\gamma} & (s \neq 0) \end{cases} \quad \text{(Mod. } N\text{)}, \tag{2.2}$$

where s is the distance between the two particles of interest measured in units of the cell parameter l from cell center to cell center. The ϕ potential is introduced to symmetrize the interaction around the ring for finite systems. The hard-core repulsive potential having been built into the model by the above scheme, the potential of the zeroth cell can be chosen arbitrarily for mathematical convenience. The ϕ potential satisfies the following symmetry conditions:

$$\phi_s = \phi_{s+N} = \phi_{s-N}. \tag{2.3}$$

Letting n_k represent the occupation number of the kth cell, the energy of the system is given by

$$H = \frac{1}{2m}\sum_{r=1}^{n} p_r^2 + \sum_{r=1}^{N}\sum_{s=1}^{N} n_r n_{r+s}\phi_s, \quad \left(\sum_{r=1}^{N} n_r = n\right) \tag{2.4}$$

where it is assumed that there are n particles in the system and that the total interaction energy of the system can be obtained by summing all pair-wise interactions. "Surface" terms (i.e., interactions with the boundary) do not occur by virtue of the periodic boundary conditions.

Now let the occupation number n_k be replaced by a cell occupation index $\sigma_k = 2n_k - 1$. The configurational part of the system energy can then be written as

$$U_c = \tfrac{1}{4}\sum_{r=1}^{N}{}'\sum_{s=1}^{N}{}'(1+\sigma_r)(1+\sigma_{r+s})\phi_s$$
$$= \left(N/4 + \tfrac{1}{2}\sum_{r=1}^{N}{}'\sigma_r\right)\Phi + \tfrac{1}{4}\sum_{r=1}^{N}{}'\sum_{s=1}^{N}{}'\sigma_r\sigma_{r+s}\phi_s, \quad (2.5)$$

where $\Phi = \sum_{s=1}^{N}\phi_s$, and the primed summation implies the restriction $\sum_{r=1}^{N}\sigma_r = 2n - N$.

The partition function appropriate for a system of n particles is then

$$\mathfrak{Q}_n = 1/(n!\,h^n)\int dx_1\cdots\int dx_n\int dp_1\cdots\int dp_n$$
$$\times \exp\{-\beta H(p_1,\cdots,p_n;x_1,\cdots x_n)\}$$
$$= 1/(n!\,\lambda^n)Z_n \quad (\beta = 1/kT), \quad (2.6)$$

where $\lambda = (\beta h^2/2\pi m)^{\frac{1}{2}}$ is the thermal wave length and results from the evaluation of the momentum integrals.[3] A straightforward analysis shows that for large systems the configurational part of the partition function takes the form

$$Z_n = \int dx_1\cdots\int dx_n \exp\{-\beta U_c(x_1,\cdots,x_n)\}$$
$$= n!\,l^n\sum_{\langle\sigma\rangle}\exp\{-\beta U_c(\sigma_1,\cdots,\sigma_N)\}, \quad (2.7)$$

where

$$\sum_{\langle\sigma\rangle} = \sum_{\sigma_1=-1}^{1}{}'\cdots\sum_{\sigma_N=-1}^{1}{}'.$$

The partition function is then

$$\mathfrak{Q}_n = (l/\lambda)^n\exp\{-\beta N\Phi/4\}$$
$$\times\sum_{\langle\sigma\rangle}\exp\left\{-\beta/4\left(\sum_{r,s}\sigma_r\sigma_{r+s}\phi_s + 2\Phi\sum_r\sigma_r\right)\right\} \quad (2.8)$$

Since the present investigation is concerned with systems subject to phase transitions, i.e., with systems in which the number of particles is not constant, it is preferable to deal with a grand canonical partition function. This also eliminates the awkward restriction on the sum of σ's. One then has

$$Q_N = \sum_{n=0}^{N}\xi^n\mathfrak{Q}_n, \quad \text{where} \quad \xi = \exp\{\beta g\} \quad (2.9)$$

and g is the chemical potential per particle. Writing $\xi l/\lambda = \exp\{\beta\mu\}$ and using the identity

$$n = \tfrac{1}{2}\sum_{r=1}^{N}(1+\sigma_r),$$

we obtain

$$Q_N = A_N\sum_{\{\sigma\}}\exp\left\{\sum_{r=1}^{N}\sum_{s=1}^{N}\sigma_r\sigma_{r+s}\theta_s + \nu\sum_{r=1}^{N}\sigma_r\right\}, \quad (2.10)$$

where

$$\sum_{\{\sigma\}} = \sum_{\sigma_1=-1}^{1}\cdots\sum_{\sigma_N=-1}^{1}, \quad A_N = \exp\{N(\nu-\Theta)\},$$
$$\theta_s = -\tfrac{1}{4}\beta\phi_s, \quad \Theta = \sum_{r=1}^{N}\theta_r,$$

and $\nu = \frac{1}{2}\beta(\mu - \Phi)$. The remainder of the investigation will use this form of the partition function as its point of departure. Each term in this sum of 2^N terms represents one possible configuration or microstate of the system. Since the particles comprising the fluid are indistinguishable, the probability of finding the system in a state of n observable particles is

$$W(n) = A_N Q_N^{-1}\sum_i{}'\exp\left\{\sum_{r,s}\sigma_r^i\sigma_{r+s}^i\theta_s + \nu\sum_r\sigma_r^i\right\}, \quad (2.11)$$

where σ_r^i represents the ith configuration of the rth cell and $\sum_i'$ implies a sum over all configurations consistent with the macroscopic state of the system. It is worthwhile noting that the cell structure of the system does not imply any spurious symmetry or lattice structure. The cells are used merely as a convenient mathematical artifice to establish a discrete space grid and fix the instantaneous position of the particles.

B. Multi-Dimensional Systems

The partition function of two- and three-dimensional systems with a limited number of bonds per particles is readily obtained from the preceding analysis of a one-dimensional system with all interactions active. Focussing attention first on a square array with nearest neighbor interactions only, we find that we can construct such a configuration by winding the one-dimensional chain around a three-dimensional torus (Fig. 1) and letting all interactions vanish except those between nearest neighbors in the chain and those between nearest-neighbor cells in adjacent rows. Figure 2 is a plane projection of such a configuration.

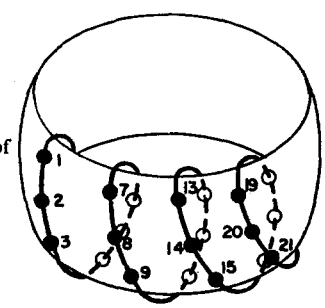

FIG. 1. Toroidal topology of 2-dimensional model.

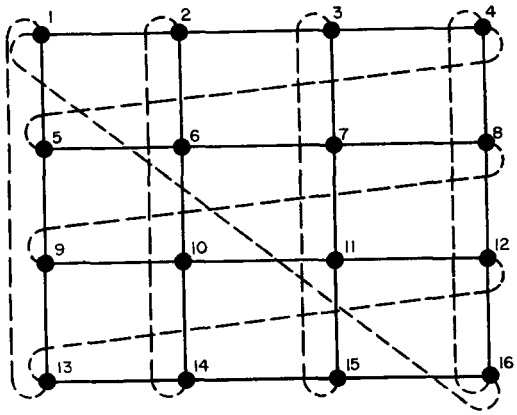

FIG. 2. Two-dimensional model in plane projection.

Thus we obtain from Eq. (2.10) the partition function for a two-dimensional square array with m cells per row simply by use of the following potential:

$$V_r = \begin{Bmatrix} -\zeta & (r = 1, m) \\ 0 & (r \neq 1, m) \end{Bmatrix} \text{(Mod. } N\text{)}, \quad (2.12)$$

with ϕ_r given by Eq. (2.3) as before. It is obvious that this potential introduces certain spurious interactions. In Fig. 2 these are shown by broken lines. While such interactions are significant in finite models, they become negligible in the thermodynamic limit. One can proceed in exactly the same way to obtain the partition function of a three-dimensional system. A typical square array of 64 cells is shown in Fig. 3. For a cubic array of N cells with m cells per row, k cells per layer, the appropriate nearest-neighbor

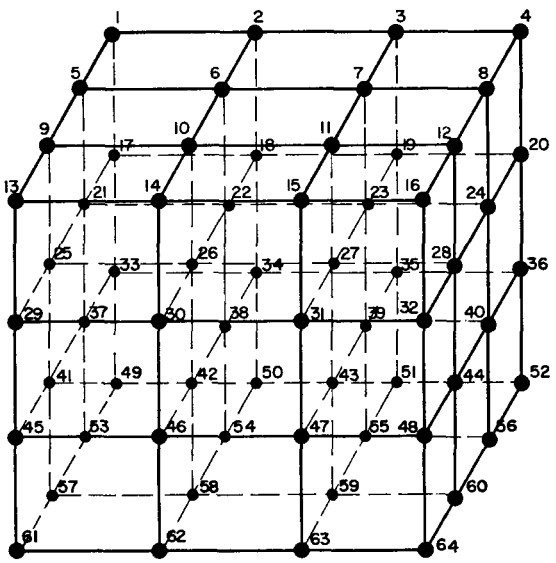

FIG. 3. Three-dimensional array.

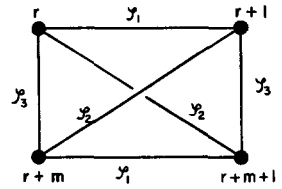

Fig. 4. Anisotropic nearest-neighbor and next-nearest-neighbor interaction.

interaction potential is

$$V_r = \begin{Bmatrix} -\zeta & (r = 1, m, k) \\ 0 & (r \neq 1, m, k) \end{Bmatrix} \text{(Mod. } N\text{)}. \quad (2.13)$$

Extension of the one-dimensional system partition function to higher dimensions is not restricted to nearest-neighbor interactions. More complicated interactions can also be accommodated, provided only that the number of bonds per cell remains finite and sufficiently small to make the analysis feasible mathematically. An element of a typical anisotropic square array with nearest-neighbor and next-nearest-neighbor interactions is shown in Fig. 4. The partition function of such a system can be obtained from Eq. (2.10) by means of the following potential:

$$V_r = \begin{Bmatrix} -\zeta_1 & (r = 1), \\ -\zeta_2 & (r = m - 1, m + 1), \\ -\zeta_3 & (r = m), \\ 0 & (r \neq 1, m - 1, m, m + 1), \end{Bmatrix} \text{(Mod. } N\text{)}. \quad (2.14)$$

In two- and three-dimensional systems, just as in one dimension, the cell structure serves merely as a space grid for the purpose of specifying the instantaneous location of the particles with an uncertainty equal to the cell dimension. To take account of the change in the momentum integrals in multidimensional systems, the parameter λ must, of course, be redefined as follows: $\lambda = (\beta h^2/2\pi m)^{d/2}$, where d is the dimensionality of the system.

C. Multiple Cell Occupancy

One can readily extend the model to take account of cell occupancies other than 0 and 1, provided that intermediate occupancies are not considered. If, for instance, one limits cell occupancy to 0 or m particles, the partition function takes the same form as Eq. (2.10) if one makes the following definitions:

ϕ_0 = average interaction potential of particles in the same cell,

$$\theta_s = -\tfrac{1}{4}\beta m^2 \phi_s; \quad \Theta' = \sum_{r=1}^{N-1} \theta_r,$$

$$v = \tfrac{1}{2}\beta m[\mu + \tfrac{1}{2}(1 + m)\phi_0 - m\Phi],$$

$$A_N = \exp\{N(v - \Theta')\}.$$

For the simple fluid with which this investigation is concerned, such a modification is undesirable since the cell size would have to be increased, thus reducing the fineness of the space grid. In addition, the hard-core repulsive potential could not be satisfied in this case.

D. Ferromagnetic Systems

The partition function in (2.10) is identical with that of an Ising ferromagnet.[3,15] Comparison of the definitions of the various parameters for the fluid and ferromagnet yields the well-known isomorphisms noted by Yang and Lee[5] and conveniently summarized by Huang.[3] The analysis can be broadened considerably, but this will not be done in the present context.

3. OPERATOR FORMULATION

Let μ_i be a state vector representing the state of the ith cell and Z be an operator defined as follows:

$$Z\mu_i = \sigma_i\mu_i. \tag{3.1}$$

We define now a vector ψ^α representing the αth configuration of the system:

$$\psi^\alpha = |\mu_1^\alpha, \mu_2^\alpha, \cdots, \mu_N^\alpha\rangle. \tag{3.2}$$

A convenient representation of ψ^α is a 2^N-dimensional one in which it is the direct product of the N two-dimensional μ-spinors. A corresponding operator Z_k can be defined in the same space as follows:

$$Z_k\psi^\alpha = \sigma_k^\alpha\psi^\alpha. \tag{3.3}$$

In the 2^N-dimensional representation the operator Z_k takes the form

$$Z_k = I \otimes I \otimes \cdots \otimes I \otimes \underset{\substack{\uparrow \\ k\text{th factor}}}{Z} \otimes I \otimes \cdots \otimes I, \tag{3.4}$$

where the I's are the two-dimensional identity. It is easy to show that in terms of these operators the partition function, Eq. (2.10), can be written as

$$Q_N = A_N\sum_{\alpha=1}^{2^N}\psi^{\alpha\dagger}S\psi^\alpha = A_N T_r(S), \tag{3.5}$$

where

$$S = S_1S_2,$$
$$S_1 = \prod_{r=1}^{N} S_{1r} = \prod_{r=1}^{N}\exp\left\{\sum_{s=1}^{N} Z_rZ_{r+s}\theta_s\right\},$$
$$S_2 = \prod_{r=1}^{N} S_{2r} = \prod_{r=1}^{N}\exp\{\nu Z_r\}.$$

The partition functions for small systems are readily computed from Eq. (3.5). Such partition functions are tabulated in Appendix A. In attempting a closed-form solution of the problem it seems natural to follow the approach of Kaufman and Onsager,[7,8] setting $S_2 = 1$ initially. It is obvious that this will not be easy since the preceding analysis shows that the general one-dimensional system considered here contains the unsolved three-dimensional Ising model as a particular subset. The analysis is outlined in Appendix B and shows that the operator S_1 is not the spin representative of commuting rotations, as it is for a two-dimensional square lattice, but is rather part of a tensor transformation. It does not appear feasible therefore to determine the eigenvalues of S in this way.

4. EVALUATION OF THE PARTITION FUNCTION

In the partition function, Eq. (3.5), consider the exponent

$$U = \sum_{r=1}^{N}\sum_{s=1}^{N} Z_rZ_{r+s}\theta_s + \nu\sum_{r=1}^{N} Z_r.$$

This can be written in the form $U = Y^\dagger\Phi Y + \Phi_0$, where $Y = \zeta - \zeta_0$, $\zeta = |Z_1, Z_2, \cdots, Z_N\rangle$, ζ_0 is a constant vector yet to be determined, Φ_0 is a scalar, also as yet undetermined, and Φ is a doubly-cyclic matrix[16]:

$$\Phi = \begin{pmatrix} 0 & \theta_1 & \theta_2 & \theta_3 & \cdots & \theta_3 & \theta_2 & \theta_1 \\ \theta_1 & 0 & \theta_1 & \theta_2 & \cdots & \theta_4 & \theta_3 & \theta_2 \\ \cdot & & & & & & & \cdot \\ \cdot & & & & & & & \cdot \\ \cdot & & & & & & & \cdot \\ \theta_1 & \theta_2 & \theta_3 & \theta_4 & \cdots & \theta_2 & \theta_1 & 0 \end{pmatrix}; \tag{4.1}$$

i.e., $\Phi_{ij} = \theta_{j-i}$ (we must remember that $\theta_{N-r} = \theta_r$). One finds readily that V_k, the kth normalized eigenvector of Φ, is given by $V_k = 1/N^{\frac{1}{2}}\omega_{k(l-1)}$, where $\omega_{kl} = \exp\{2\pi kli/N\}$, while the kth eigenvalue is

$$\lambda_k = \sum_{r=1}^{N}\cos[(2\pi/N)kr]\theta_r.$$

The λ's are thus the finite Fourier cosine transforms of the θ potentials. The matrix Φ being symmetric, its eigenvectors form, of course, an orthonormal set. We now make the following identifications:

$$\zeta^\dagger\Phi\zeta = \sum_{r=1}^{N}\sum_{s=1}^{N} Z_rZ_{r+s}\theta_s, \quad \zeta^\dagger\Phi\zeta_0 + \zeta_0^\dagger\Phi\zeta = -\nu\sum_{r=1}^{N} Z_r, \tag{4.2}$$
$$\Phi_0 = -\zeta_0^\dagger\Phi\zeta_0.$$

[15] S. Fluegge, *Handbuch der Physik* (Springer-Verlag, Berlin, 1962), Vol. XIII.

[16] The symbols $\Phi, \Phi_0, \zeta, \zeta_0$, and V_k have the meaning defined here only in the present section and must not be confused with the corresponding symbols used elsewhere in this paper.

One shows easily that $\zeta_0 = aV_N$, while

$$a = -N^{\frac{1}{2}}\nu/2\lambda_N.$$

The partition function then takes the form

$$Q_N = B_N \operatorname{Tr} [\exp \{Y^\dagger \Phi Y\},$$
$$B_N = A_N \exp \{-a^2\lambda_N\}]. \tag{4.3}$$

The quadratic form $Y^\dagger \Phi Y$ can be diagonalized in the usual way by letting $Y = S\eta$, where S is an $N \times N$ matrix whose columns are the eigenvectors of Φ. Then we have that

$$Y^\dagger \Phi Y = \sum_{r=1}^{N} |\eta_r|^2 \lambda_r.$$

Remembering that the η's are operators, we determine their eigenvalues from the following equation:

$$\begin{aligned}\eta_r \psi^\alpha &= \left[1/N^{\frac{1}{2}} \sum_{s=1}^{N} \omega_{-r(s-1)} Z_s - a\delta_{r,N}\right]\psi^\alpha \\ &= \left[1/N^{\frac{1}{2}} \sum_{s=1}^{N} \omega_{-r(s-1)} \sigma_s^\alpha - a\delta_{r,N}\right]\psi^\alpha \\ &= \chi_r^\alpha \psi^\alpha. \end{aligned} \tag{4.4}$$

The partition function can then be written as follows:

$$\begin{aligned} Q_N &= B_N \operatorname{Tr} \left[\exp \left\{\sum_{r=1}^{N} |\eta_r|^2 \lambda_r\right\}\right] \\ &= B_N \sum_{\{C_i\}} g(C_i) \exp \left\{\sum_{r=1}^{N} |\chi_r(C_i)|^2 \lambda_r\right\}. \end{aligned} \tag{4.5}$$

The sum in the last equation is over all macroscopic configurations, $g(C_i)$ being the degeneracy of the ith such configuration, i.e., the number of microstates corresponding to the ith macrostates. It proves most convenient to choose as the macroscopic configurations appearing in the sum the number of particles (n) in the system. The sum can then be carried out in terms of successive deviations from the perfectly ordered state. One readily shows that $|\chi_r|^2$ is given by

$$|\chi_r(n)|^2 = \begin{cases} 4/N \sum_{i=1}^{n} \sum_{j=1}^{n} \cos [2\pi/Nr(q_i - q_j)] & (r \neq N), \\ (N + aN^{\frac{1}{2}} - 2n)^2/N & (r = N), \end{cases} \tag{4.6}$$

where it was assumed that the occupied cells are cells q_1 through q_n. One finds that this expression is invariant to the substitution $n \to N - n$; i.e., Eq. (4.6) is the same for a system of n occupied or n empty cells, $|\chi_r(n)|^2 = |\chi_r(N-n)|^2$. Before the sum in Eq. (4.5) can be carried out, a consistency condition must be satisfied. This results from the fact that

$$\psi^{\alpha\dagger} \psi^\alpha = \sum_{r=1}^{N} (\sigma_r^\alpha)^2 = N.$$

The consistency condition here is

$$\chi^\dagger \chi = N - 4an/N^{\frac{1}{2}} + 2aN^{\frac{1}{2}} + a^2.$$

One can give this condition a geometrical interpretation. The original sum in the partition function in terms of the σ's can be thought of as a sum over the corners of an N-dimensional cube having sides two units in length. The transformation used above to diagonalize the quadratic form $Y^\dagger \Phi Y$ rotates the coordinate system and translates the origin. The consistency condition then states that distances must remain invariant under this transformation. One readily verifies that every term in the expansion of Eq. (4.5) satisfies this condition. Carrying out the sum in (4.5) in terms of successive deviations from the perfectly ordered state, after some simplification and rearrangement one obtains

$$Q_N = 2C_N \sum_{n=0}^{[N/2]} T_n, \quad C_N = \begin{cases} \exp \{N\nu\} & \text{(fluid)}, \\ \exp \{N\Theta\} & \text{(ferromagnet)}, \end{cases} \tag{4.7}$$

$$T_n = \cosh [(N - 2n)\nu] X^{-n/2} t_n (1 - \tfrac{1}{2}\delta_{n,N/2}),$$
$$t_n = (1/n!) \sum_{q_1=1}^{N}{}' \cdots \sum_{q_n=1}^{N}{}' \prod_{r=1}^{n} \prod_{s=1}^{n} x_{(q_r - q_s)},$$
$$x_r = \exp \{8\theta_r\}, \quad X = \prod_{r=1}^{N} x_r.$$

The primed sums indicate that no index may be repeated in any one term, while $[m]$ means "nearest integer equal to or less than m."

5. CONVERGENCE AND ANALYTICITY

A. Convergence

As long as N is finite, the series in Eq. (4.7) obviously converges, so that the question of convergence is of interest only in the thermodynamic limit, i.e., as $N \to \infty$. Convergence of the series in that limit depends on the sign of the exponent

$$4\left[\sum_{r=1}^{n} \sum_{s=1}^{n} \theta_{(q_r - q_s)} - n\Theta\right] = 4\left[\sum_{r=1}^{n} \sum_{s=1}^{n} \theta_{(q_r - q_s)} - n \sum_{r=1}^{N} \theta_r\right]. \tag{5.1}$$

Remembering that in the limit $N \to \infty$ symmetries due to boundary conditions disappear, we find that none of the θ's in the double sum occur with a multiplicity greater than $(n - 1)$. Hence for any attractive interaction with hard core (not necessarily a Lennard-Jones potential) the expression in (5.1) is less than zero (since $\theta_r \geq 0$, $\forall r$). For example, for a potential of constant depth ϵ, expression (5.1) is

$4n(n-N)\epsilon \leq 0$, since $\epsilon \geq 0$ and $0 \leq n \leq N/2$. Thus we have

$$0 \leq \cosh(N\nu) + \sum_{n=1}^{[N/2]} 1/n!\cosh[(N-2n)\nu] \times \sum_{q_1=1}^{N}{}' \cdots \sum_{q_n=1}^{N}{}' \exp\left\{4\left[\sum_{r=1}^{n}\sum_{s=1}^{n}\theta_{q_r-q_s} - n\Theta\right]\right\}(1-\tfrac{1}{2}\delta_{n,N/2}) \leq \tfrac{1}{2}\exp\{N\nu\}\sum_{n=0}^{N}\binom{N}{n}\exp\{-2n\nu\} = 2^{N-1}\cosh^N\nu. \tag{5.2}$$

Hence

$$0 \leq Q_N(\nu,\theta) \leq 2^N C_N \cosh^N\nu = \begin{cases}(1+\exp\{2\nu\})^N & \text{(fluid)},\\ 2\exp\{N\Theta\}\cosh^N\nu & \text{(ferromagnet)}.\end{cases} \tag{5.3}$$

Consequently,

$$0 \leq \lim_{N\to\infty} Q_N^{1/N} \leq \begin{cases}(1+\exp\{2\nu\}) & \text{(fluid)},\\ 2\exp\{\Theta\}\cosh\nu & \text{(ferromagnet)}.\end{cases} \tag{5.4}$$

The series in Eq. (4.7) therefore has the following properties:

(1) $\lim_{N\to\infty} Q_N^{1/N}$ exists;

(2) $q = \lim_{N\to\infty}(1/N)\ln(Q_N)$ exists;

(3) The series representing these functions are absolutely and uniformly convergent for all finite values of the parameter ν.

B. Analyticity

The partition function of Eq. (4.7) can be written in the form

$$Q_N = 2C_N\sum_{n=0}^{[N/2]} a_n\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}) = C_N\begin{cases}y^{-N/2}P_N(\Theta,y) & (y\leq 1),\\ y^{N/2}P_N(\Theta,y^{-1}) & (y>1),\end{cases} \tag{5.5}$$

where

$$P_N(\Theta,y) = \sum_{n=0}^{N} a_n y^n, \quad y = \exp\{2\nu\},$$

$$a_n = (1/n!)X^{-n/2}\sum_{q_1=1}^{N}{}'\cdots\sum_{q_n=1}^{N}{}'\prod_{\substack{r=1\\(r<s)}}^{n}\prod_{s=1}^{n} x_{q_r-q_s}.$$

It is readily shown that the coefficients have the following properties:

$$a_n = a_n^*, \quad a_n \leq \binom{N}{n}, \quad a_n = a_{N-n}, \quad a_n \geq 0, \quad a_0 = 1. \tag{5.6}$$

Since $C_N = y^{N/2}$ for a fluid, we see that the partition function is analytic throughout the entire finite complex y plane, but has a pole of order N at the ideal point at infinity. This agrees with physical reasoning, since the point $y = 0$ corresponds to a system of zero density, while $y \to \infty$ represents a system in which every cell is filled, i.e., of density $\rho = 1$, where ρ is defined as[17]

$$\rho = \langle n\rangle/N. \tag{5.7}$$

Conversely, a ferromagnet has poles of order $N/2$ at the origin and at infinity, corresponding to a diverging free energy at these points. This behavior is again what one would expect on physical grounds since these points represent an infinitely large external magnetic field aligned with the negative and positive z axis, respectively.

In view of the connection established by Yang and Lee between phase changes and zeros of the partition function,[5] the distribution of these zeros is of particular interest. One concludes from Eq. (5.5) that the zeros of Q_N coincide with those of the polynomial P_N. It is apparent from Eq. (5.5) and the properties of the coefficients in Eq. (5.6) that the roots occur in complex conjugate pairs and inverse pairs; i.e., if y_k is such a root, then y_k^*, y_k^{-1}, and $(y_k^*)^{-1}$ are roots also. Furthermore, no roots can lie on the positive real axis for any finite N. Using Yang and Lee's result that $|y_k| \leq 1$, it follows at once that all roots must lie on the unit circle in the complex y plane. Furthermore, if N is odd, at least one of the roots must lie at $y = -1$.

The analysis can be carried considerably further; this will be done in a later publication.

6. NEAREST-NEIGHBOR APPROXIMATIONS

In this section the series form of the partition function in Eq. (4.7) will be applied to one-, two-, and three-dimensional systems with nearest-neighbor interactions. In the one-dimensional case the solution so obtained can be checked against the known closed-form solution to establish the validity of the present approach and to develop the algebraic machinery for two- and three-dimensional low-temperature series approximations.

[17] It will be shown in the second of this series [J. Math. Phys. **9**, 1957 (1968), following paper] that the density ρ is given by $\rho = (\frac{1}{2})(1 + T_\nu/NT)$, where

$$T_\nu = \sum_{n=0}^{[N/2]}(N-2n)\cdot\sinh[(N-2n)\nu]X^{-n/2}t_n(1-\tfrac{1}{2}\delta_{n,N/2})$$

and

$$T = \sum_{n=0}^{[N/2]}\cosh[(N-2n)\nu]\cdot X^{-n/2}t_n(1-\tfrac{1}{2}\delta_{n,N/2}).$$

Hence for $\nu \to -\infty$ or $y = 0$, $\rho = 0$; while for $\nu \to +\infty$ or $\nu \to +\infty$, $\rho = 1$,

A. One-Dimensional System

The potential to be used is

$$V_r = \begin{cases} -\zeta & (r = 1), \\ 0 & (r \neq 1). \end{cases} \tag{6.1}$$

Then

$$X_r = \exp\{4\epsilon(\delta_{r,1} + \delta_{r,N-1})\} = 1 + a\Delta_r, \tag{6.2}$$

where

$$\epsilon = 2\theta_1 = \tfrac{1}{4}\beta\zeta, \quad a = X_1 - 1,$$
$$\Delta_r = \delta_{r,1} + \delta_{r,N-1} \text{ (modulo } N).$$

We can now evaluate the partition function term by term. Thus [cf. Eq. (4.7)]

$$t_0 = 1, \quad t_1 = \sum_{q=1}^{N} \cdot 1 = N, \tag{6.3}$$

$$\begin{aligned} t_2 &= \tfrac{1}{2}\Sigma'_{q_1q_2}x_{12} = \tfrac{1}{2}\{\Sigma_{q_1q_2}x_{12} - \Sigma_{\underline{q_1q_2}}x_{12}\} \\ &= \tfrac{1}{2}\{\Sigma_{q_1q_2}(1 + a\Delta_{12}) - N\} \\ &= \tfrac{1}{2}(N^2 + 2aN - N) \\ &= (N/2)(N + 2x_1 - 3), \end{aligned}$$

where the following abbreviated notation was used:

$$\Sigma_{q_1 \cdots q_n} = \sum_{q_1=1}^{N} \cdots \sum_{q_n=1}^{N}, \quad x_{ij} = x_{q_i - q_j}, \quad \Delta_{ij} = \Delta_{q_i - q_j} \tag{6.4}$$

and

$$\Sigma_{\underline{q_1q_2}}x_{12} = \Sigma_{q_1q_2}x_{12}\delta_{q_1,q_2}.$$

For the next term in the expansion we find

$$\begin{aligned} t_3 &= 1/(3!)\,\Sigma'_{q_1q_2q_3}x_{12}x_{13}x_{23} \\ &= 1/(3!)\,\Sigma_{q_1q_2q_3}(1 + a\Delta_{12})(1 + a\Delta_{13})\cdot(1 + a\Delta_{23}) \\ &\qquad \times (1 - \delta_{q_1,q_2})(1 - \delta_{q_1,q_3})(1 - \delta_{q_2,q_3}) \\ &= 1/(3!)\,\{\Sigma_{q_1q_2q_3} - 3\Sigma_{\underline{q_1q_2}q_3} + 2\Sigma_{\underline{q_1q_2q_3}}\}(1 + a\Delta_{12}) \\ &\qquad \times (1 + a\Delta_{13})(1 + a\Delta_{23}) \\ &= (N/3!)[6x_1^2 + 6(N - 4)x_1 + (N - 4)(N - 5)]. \end{aligned} \tag{6.5}$$

In arriving at this result the following was used:

$$\Sigma_{q_1q_2q_3}\Delta_{12}\Delta_{13}\Delta_{23} = 0, \tag{6.6}$$

which follows directly if one notes that all δ-function products occurring in this sum are incompatible. If one associates with each Δ function the corresponding Boltzmann factor x_1, or, equivalently, the corresponding a factor, one can think of the function Δ_{ij} as a bond between cells q_i and q_j. From that point of view, which will be useful in evaluating higher terms, one can say that any triangular configuration of bonds makes a vanishing contribution to the partition function. This result is readily generalized: Any configuration of bonds which includes a closed multilateral with an odd number of sides makes a vanishing contribution to the partition function.

In expanding the primed sums in t_4, one obtains

$$\begin{aligned} t_4 &= (1/4!)\Sigma'_{q_1q_2q_3q_4}x_{12}x_{13}x_{14}x_{23}x_{24}x_{34} \\ &= (1/4!)\{\Sigma_{q_1q_2q_3q_4} - 6\Sigma_{\underline{q_1q_2}q_3q_4} + 8\Sigma_{\underline{q_1q_2q_3}q_4} \\ &\qquad + 3\Sigma_{\underline{q_1q_2}\,\underline{q_3q_4}} - 6\Sigma_{\underline{q_1q_2q_3q_4}}\}x_{12}x_{13}x_{14}x_{23}x_{24} \\ &= (1/4!)\Bigg\{\Sigma_{q_1q_2q_3q_4}\prod_{\substack{r=1 \\ s=1 \\ (r<s)}}^{4}(1 + a\Delta_{rs}) \\ &\qquad - 6\Sigma_{q_1q_2q_3}(1 + a\Delta_{12})^2(1 + a\Delta_{13})^2\cdot(1 + a\Delta_{23}) \\ &\qquad + \Sigma_{q_1q_2}[8(1 + a\Delta_{12})^3 + 3(1 + a\Delta_{12})^4] - 6N\Bigg\}. \end{aligned} \tag{6.7}$$

The sums are easily evaluated except for the first one where the algebra becomes somewhat tedious. It can be simplified considerably by determining the number of ways of distributing one, two, . . . , six bonds among four cells. In this way, for the entire term one has

$$\begin{aligned} t_4 &= (N/4!)[24x_1^3 + 36(N - 5)x_1^2 \\ &\qquad + 12(N - 5)(N - 6)x_1 + (N - 5)(N - 6) \\ &\qquad \times (N - 7)]. \end{aligned} \tag{6.8}$$

In evaluating t_5 the following result is helpful:

$$\sum_{k=1}^{m}\binom{m}{k}a^k = \sum_{k=1}^{m}\sum_{l=0}^{k}\binom{m}{k}\binom{k}{l}(-1)^{k-l}x_1^l = x_1^m - 1. \tag{6.9}$$

Expansion of the primed sums yields

$$\begin{aligned} t_5 &= 1/(5!)\Sigma'_{q_1 \cdots q_5}\prod_{\substack{r=1 \\ s=1 \\ (r<s)}}^{5}x_{rs} \\ &= 1/(5!)\Sigma_{q_1 \cdots q_5} - 10\Sigma_{\underline{q_1q_2}q_3q_4q_5} \\ &\quad + 15\Sigma_{\underline{q_1q_2}\,\underline{q_3q_4}q_5} + 20\Sigma_{\underline{q_1q_2q_3}q_4q_5} - 20\Sigma_{\underline{q_1q_2}q_3\underline{q_4q_5}} \\ &\quad - 30\Sigma_{\underline{q_1q_2q_3q_4}q_5} + 24\Sigma_{\underline{q_1q_2q_3q_4q_5}}\}\prod_{\substack{r=1 \\ s=1 \\ (r<s)}}^{5}x_{rs} \\ &= 1/(5!)\Bigg\{\Sigma_{q_1 \cdots q_5}\prod_{\substack{r,s=1 \\ (r<s)}}^{5}(1 + a\Delta_{rs}) \\ &\quad - 10\Sigma_{q_1q_2q_3q_4}(1 + a\Delta_{12})^2(1 + a\Delta_{13})^2 \\ &\quad \times (1 + a\Delta_{14})^2(1 + a\Delta_{23})(1 + a\Delta_{24})(1 + a\Delta_{34}) \\ &\quad + \Sigma_{q_1q_2q_3}[15(1 + a\Delta_{12})^4\cdot(1 + a\Delta_{13})^2(1 + a\Delta_{23})^2 \\ &\quad + 20(1 + a\Delta_{12})^3(1 + a\Delta_{13})^3(1 + a\Delta_{23})] \\ &\quad - \Sigma_{q_1q_2}[20(1 + a\Delta_{12})^6 + 30(1 + a\Delta_{12})^4] + 24N\Bigg\}. \end{aligned} \tag{6.10}$$

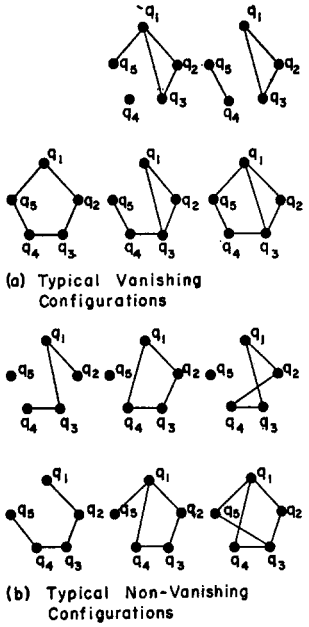

FIG. 5. Typical bond configurations for t_5.

The sums occurring here are identical with those encountered in previous terms and are evaluated in the same way except for the first one. In carrying out the first sum one observes that it can be decomposed into ten equivalent single-bond terms, 45 equivalent two-bond terms, 120 triple-bond terms of which ten include triangular bond configurations and therefore vanish, etc. Figure 5 shows some typical vanishing and nonvanishing bond configurations occurring in this sum. Reasoning in this way, one finds

$$\begin{aligned}
&\Sigma_{q_1q_2q_3q_4q_5}\prod_{\substack{r,s=1\\(r<s)}}^{5}(1+a\Delta_{rs})\\
&=\Sigma_{q_1\cdots q_5}\{1+10a\Delta_{12}+45a^2\Delta_{12}\Delta_{13}\\
&\quad+110a^3\Delta_{12}\Delta_{13}\Delta_{14}+15a^4\Delta_{12}\Delta_{23}\Delta_{34}\Delta_{14}\\
&\quad+125a^4\Delta_{12}\Delta_{23}\Delta_{34}\Delta_{45}+60a^5\Delta_{12}\Delta_{23}\Delta_{34}\\
&\quad\times\Delta_{14}\Delta_{15}+10a^6\Delta_{12}\Delta_{14}\Delta_{15}\Delta_{23}\Delta_{34}\Delta_{35}+\text{zero terms}\}\\
&=N[N^4+20N^3(x_1-1)+180N^2(x_1^2-2x_1+1)\\
&\quad+10N(9x_1^4+52x_1^3-210x_1^2+228x_1-79)\\
&\quad+20(5x_1^6+6x_1^5-5x_1^4-140x_1^3\\
&\quad+315x_1^2-250x_1+69].
\end{aligned}\tag{6.11}$$

For the entire term one finds

$$\begin{aligned}
t_5=(N/5!)[&120x_1^4+240(N-6)x_1^3\\
&+120(N-6)(N-7)x_1^2\\
&+20(N-6)(N-7)(N-8)x_1\\
&+(N-6)(N-7)(N-8)(N-9)].
\end{aligned}\tag{6.12}$$

Combining these results, for the one-dimensional partition function correct to this term one has

$$\begin{aligned}
Q_N=2C_N\{&\cosh(N\nu)+Nx_1^{-1}\cosh[(N-2)\nu]\\
&+(N/2)x_1^{-2}(2x_1+N-3)\cosh[(N-4)\nu]\\
&+(N/3!)x_1^{-3}[6x_1^2+6(N-4)x_1\\
&+(N-4)(N-5)]\cosh[(N-6)\nu]\\
&+(N/4!)x_1^{-4}[24x_1^3+36(N-5)x_1^2\\
&+12(N-5)(N-6)x_1\\
&+(N-5)(N-6)(N-7)]\cosh[(N-8)\nu]\\
&+(N/5!)x_1^{-5}[120x_1^4+240(N-6)x_1^3\\
&+120(N-6)(N-7)x_1^2\\
&+20(N-6)(N-7)(N-8)x_1\\
&+(N-6)(N-7)(N-8)(N-9)]\\
&\times\cosh[(N-10)\nu]+\cdots\}.
\end{aligned}\tag{6.13}$$

Equation (6.13) suggests strongly that one should be able to write the one-dimensional partition function in the following form:

$$Q_N=2C_N\sum_{n=0}^{[N/2]}x_1^{-n}t_n\cosh[(N-2n)\nu(1-\tfrac{1}{2}\delta_{n,N/2}),\tag{6.14}$$

where

$$t_n=\begin{cases}1 & (n=0),\\ \dfrac{N}{n}\displaystyle\sum_{k=1}^{n}\binom{n}{k}\binom{N-n-1}{k-1}x_1^{n-k} & (n\neq 0).\end{cases}$$

One can re-express t_n in the form

$$\begin{aligned}
t_n&=\frac{N}{n}\sum_{k=1}^{n}\binom{n}{k}\binom{N-n-1}{k-1}(1+a)^{n-k}\\
&=\frac{N}{n}\sum_{l=0}^{n-1}\sum_{k=1}^{n-l}\binom{n}{k}\binom{N-n-1}{k-1}\binom{n-k}{l}a^l\quad(n\neq 0).
\end{aligned}\tag{6.15}$$

Conversely, from Eqs. (4.7) and (6.2) one has that

$$t_n=(1/n!)\Sigma'_{q_1}\cdots{}_{q_n}\prod_{\substack{r,s=1\\(r<s)}}^{n}(1+a\Delta_{rs})\quad(n\neq 0).\tag{6.16}$$

If Eq. (6.14) is to be correct, then these two expressions for t_n must be equal. While an explicit proof of this equality does not seem feasible, the coefficients of a were determined from these two expressions for a wide range of N and n by computer. The equality of the coefficients in all cases examined presents persuasive evidence that the formulation of the partition function in Eq. (6.14) is in fact correct.

It is possible to carry out the sum in Eq. (6.14), thus obtaining a closed-form solution for the one-dimensional nearest-neighbor model which agrees with the solution found by other methods. This analysis is carried out in Appendix C, where it is shown that

the partition function of such a system has the form

$$Q_N = C_N \cosh^N(\nu)\{(1+(1+\omega)^{\frac{1}{2}})^N + (1-(1+\omega)^{\frac{1}{2}})^N\},$$
$$C_N = \begin{cases}\exp\{N\nu\} & \text{(fluid)},\\ \exp\{N\epsilon\} & \text{(ferromagnet)},\end{cases} \qquad (6.17)$$
$$\omega = (x_1^{-1}-1)\operatorname{sech}^2\nu.$$

Agreement with the known solution of this model establishes the validity of the present approach as a preliminary to applying this method to systems of higher dimensions.[18]

B. Multi-Dimensional Systems

Considering now two- and three-dimensional systems of N cells, the appropriate potentials are those of Eqs. (2.12) and (2.13), respectively. The definitions of Eq. (6.2) then change as follows:

$$\epsilon = \tfrac{1}{4}\beta\zeta = \begin{cases}2\theta_1 = 2\theta_m = 2\theta_{N-1} = 2\theta_{N-m} & \text{(2-dim. system)},\\ 2\theta_1 = 2\theta_m = 2\theta_k = 2\theta_{N-1} = 2\theta_{N-m} = 2\theta_{N-k} & \text{(3-dim. system)},\end{cases} \qquad (6.18)$$

$$\Delta_r = \begin{cases}\delta_{r,1}+\delta_{r,m}+\delta_{r,N-1}+\delta_{r,N-m} & \text{(2-dim. system)},\\ \delta_{r,1}+\delta_{r,m}+\delta_{r,k}+\delta_{r,N-1}+\delta_{r,N-m}+\delta_{r,N-k} & \text{(3-dim. system)}.\end{cases}$$

The change in definition of the Δ functions reflects, of course, the change in coordination number of the system. One can now proceed to determine the terms in the series expansion of the partition function algebraically in exactly the same way as in the one-dimensional case. The expansions of the primed sums occurring in t_n remain unchanged, as do the coefficients (expressed in series form) of the various powers of a. Indeed, there are only two changes in this entire process. One is the changed value of X defined in Eq. (4.7):

$$X = \prod_{r=1}^{N} x_r = \prod_{r=1}^{N}(1+a\Delta_r) = \begin{cases}x_1^2 & \text{(1-dim. system)},\\ x_1^4 & \text{(2-dim. system)},\\ x_1^6 & \text{(3-dim. system)}.\end{cases} \qquad (6.19)$$

Secondly, the value of sums of Δ-function products changes because of the changed definition of Δ_r. This causes a change in the actual numerical value of the coefficients of a. Table I shows the values of typical such sums. These changes are sufficient, of course, to modify the actual terms in the series materially. As a typical example, one finds that the fourth term in the series expansion is given by

$$T_4 = \cosh[(N-8)\nu]t_4(1-\tfrac{1}{2}\delta_{4,N/2}) \times \begin{cases}x_1^{-2} & \text{(1-dim. system)},\\ x_1^{-8} & \text{(2-dim. system)},\\ x_1^{-12} & \text{(3-dim. system)},\end{cases} \qquad (6.20)$$

$$t_4 = 1/(4!)\Sigma'_{q_1q_2q_3q_4}\prod_{\substack{r,s=1\\(r<s)}}^{4}(1+a\Delta_{rs}) = \Big\{1/(4!)\Sigma_{q_1q_2q_3q_4} - 6\Sigma_{\underline{q_1q_2}q_3q_4} + 8\Sigma_{\underline{q_1q_2q_3}q_4} + 3\Sigma_{\underline{q_1q_2}\underline{q_3q_4}} - 6\Sigma_{\underline{q_1q_2q_3q_4}}\Big\}\prod_{\substack{r,s=1\\(r<s)}}^{4}(1+a\Delta_{rs})$$
$$= 1/(4!)\{\Sigma_{q_1q_2q_3q_4}[1+6a\Delta_{12}+15a^2\Delta_{12}\Delta_{13}+16a^3\Delta_{12}\Delta_{13}\Delta_{14}+4a^3\Delta_{12}\Delta_{13}\Delta_{23}+12a^4\Delta_{12}\Delta_{13}\Delta_{14}\Delta_{34}+3a^4\Delta_{12}\Delta_{23}\Delta_{34}\Delta_{14}] - 6\Sigma_{q_1q_2q_3}[1+(3+2a)a\Delta_{12}+(4+4a+a^2)a^3\Delta_{12}\Delta_{13}\Delta_{23}] + \Sigma_{q_1q_2}[11+(36+42a+20a^2+3a^3)\times a\Delta_{12}]-6N\},$$
$$= \frac{N}{4!}\begin{cases}[24x_1^3+36(N-5)x_1^2+12(N-5)(N-6)x_1+(N-5)(N-6)(N-7)] & \text{(1-dim. system)},\\ [24x_1^4+432x_1^3+24(8N-85)x_1^2+24(N^2-21N+18)x_1+N^3-30N^2+323N-1254] & \text{(2-dim. system)},\\ [72x_1^4+1992x_1^3+36(13N-219)x_1^2+36(N^2-31N+270)x_1+N^3-42N^2+659N-3906] & \text{(3-dim. system)}.\end{cases}$$

Structuring the other terms of the partition function from the one-dimensional one in the same way, one obtains for the two-dimensional series

$$Q_N = 2C_N\{\cosh(N\nu)+Nx_1^{-2}\cosh[(N-2)\nu] + (N/2!)x_1^{-4}[4x_1+(N-5)]\cosh[(N-4)\nu] + (N/3!)x_1^{-6}[36x_1^2+12(N-8)x_1+N^2-15N+62]\cosh[(N-6)\nu] + (N/4!)x_1^{-8}[24x_1^4+432x_1^3+24(8N-85)x_1^2+24(N^2-21N+18)x_1+N^3-30N^2+323N-1254]\cosh[(N-8)\nu] + (N/5!)x_1^{-10}[960x_1^5+120(N+43)x_1^4+1200(3N-40)x_1^3+120(5N^2-132N+926)x_1^2+40(N^3-39N^2+536N-2616)x_1+N^4-50N^3+995N^2-9370N+35424]\times\cosh[(N-10)\nu]+\cdots\}. \qquad (6.21)$$

[18] Further proof of the validity of the model appears in the second article, where it is shown that for a hard-rod potential the present solution reduces correctly to the Tonks equation of state.

TABLE I. Sums of Δ-function products for systems of various dimensions.

Reference figure	Sums of Δ functions	Value of sums		
		1-Dim. system	2-Dim. system	3-Dim. system
	$\Sigma_{q_1q_2}\Delta_{12}$	$2N$	$4N$	$6N$
	$\Sigma_{q_1q_2q_3}\Delta_{12}\Delta_{13}$	$4N$	$16N$	$36N$
	$\Sigma_{q_1q_1q_3}\Delta_{12}\Delta_{13}\Delta_{23}$	0	0	0
	$\Sigma_{q_1q_2q_3q_4}\Delta_{12}\Delta_{13}\Delta_{14}$	$8N$	$64N$	$216N$
	$\Sigma_{q_1q_2q_3q_4}\Delta_{12}\Delta_{23}\Delta_{34}\Delta_{14}$	$6N$	$36N$	$90N$
	$\Sigma_{q_1q_2q_3q_4q_5}\Delta_{12}\Delta_{23}\Delta_{34}\Delta_{45}\Delta_{15}$	0	0	0
	$\Sigma_{q_1q_2q_3q_4q_5}\Delta_{12}\Delta_{14}\Delta_{15}\Delta_{23}\Delta_{34}\Delta_{35}$	$10N$	$100N$	$318N$

For the corresponding three-dimensional series one has

$$\begin{aligned}Q_N = 2C_N\{&\cosh(N\nu) + Nx_1^{-3}\cosh[(N-2)\nu]\\ &+ (N/2!)x_1^{-6}[6x_1 + (N-7)]\cosh[(N-4)\nu]\\ &+ (N/3!)x_1^{-9}[90x_1^2 + 18(N-12)x_1\\ &+ N^2 - 21N + 128]\cosh[(N-6)\nu]\\ &+ (N/4!)x_1^{-12}[72x_1^4 + 1992x_1^3\\ &+ 36(13N-219)x_1^2 + 36(N^2 - 31N + 270)x_1\\ &+ N^3 - 42N^2 + 659N - 3906]\cosh[(N-8)\nu]\\ &+ (N/5!)x_1^{-15}[5760x_1^5 + 120(3N+426)x_1^4\\ &+ 480(32N-701)x_1^3\\ &+ 360(20N^2 - 163N + 1844)x_1^2\\ &+ 60(N^3 - 57N^2 + 1190N - 9216)x_1 + N^4\\ &- 70N^3 + 2015N^2 - 28490N + 169744]\\ &\times\cosh[(N-10)\nu] + \cdots\}. \end{aligned} \tag{6.22}$$

Since one wishes eventually to go to the thermodynamic limit, it is more useful to work with a series expansion of $e^q = Q_N^{1/N}$ where q is Kramer's grand potential.[19] Using a method due to Domb,[20] one obtains the following series for a two-dimensional system from Eq. (6.21):

$$\begin{aligned}Q_N^{1/N} = C_N^{1/N}y^{-\frac{1}{2}}\{&1 + x_1^{-2}y + 2(x_1^{-3} - x_1^{-4})y^2\\ &+ 2(3x_1^{-4} - 7x_1^{-5} + 4x_1^{-6})y^3\\ &+ (x_1^{-4} + 18x_1^{-5} - 77x_1^{-6} + 98x_1^{-7} - 40x_1^{-8})y_4\\ &+ (8x_1^{-5} + 44x_1^{-6} - 370x_1^{-7} + 799x_1^{-8}\\ &- 706x_1^{-9} + 225x_1^{-10})y^5 + \cdots\}. \end{aligned} \tag{6.23}$$

For a three-dimensional system from Eq. (6.22) in the same way one has

$$\begin{aligned}Q_N^{1/N} = C_N^{1/N}y^{-\frac{1}{2}}\{&1 + x_1^{-3}y + 3(x_1^{-5} - x_1^{-6})y^2\\ &+ 3(5x_1^{-7} - 11x_1^{-8} + 6x_1^{-9})y^3\\ &+ (3x_1^{-8} + 83x_1^{-9} - 309x_1^{-10}\\ &+ 360x_1^{-11} - 137x_1^{-12})y^4\\ &+ (48x_1^{-10} + 429x_1^{-11} - 2676x_1^{-12} + 5055x_1^{-13}\\ &- 4041x_1^{-14} + 1185x_1^{-15})y^5 + \cdots\}. \end{aligned} \tag{6.24}$$

These series are valid for $y \leq 1$. Corresponding series for $y > 1$ can be obtained by the simple transformation of Eq. (5.5). It is also possible to obtain from (6.21) or (6.22) a series for the grand potential. Thus, for the three-dimensional system one has

$$\begin{aligned}q &= \beta\rho\ell\\ &= \lim_{N\to\infty}(1/N)\ln Q_N\\ &= 1 + x_1^{-3}y + (3x_1^{-5} - \tfrac{7}{2}x_1^{-6})y^2\\ &\quad + (15x_1^{-7} - 36x_1^{-8} + 21\tfrac{1}{3}x_1^{-9})y^3\\ &\quad + (3x_1^{-8} + 83x_1^{-9} - 328\tfrac{1}{2}x_1^{-10}\\ &\quad + 405x_1^{-11} - 162\tfrac{3}{4}x_1^{-12})y^4\\ &\quad + (48x_1^{-10} + 426x_1^{-11} - 2804x_1^{-12} + 5532x_1^{-13}\\ &\quad + 4608x_1^{-14} + 1406\tfrac{1}{5}x_1^{-15})y^5 + \cdots. \end{aligned} \tag{6.25}$$

As mentioned in Sec. 4, these series represent successive deviations from the perfectly ordered state and hence are in fact low-temperature expansions. Comparison with similar series computed by others using entirely different techniques shows complete agreement insofar as the terms overlap and after making allowance for differences in notation.[20–22] This serves to confirm the validity of the transformation discussed

[19] D. ter Haar, *Elements of Statistical Mechanics* (Holt, Rinehart and Winston, New York, 1964).
[20] C. Domb, Adv. Phys. 9, 149 (1960).
[21] A. J. Wakefield, Proc. Cambridge Phil. Soc. 47, 419, 799 (1951).
[22] S. G. Brush, "History of the Lenz–Ising Model," University of California, Lawrence Radiation Laboratory Report UCRL-7940, 1964.

in Sec. 2, whereby a one-dimensional system with all interactions active can be converted to a system of higher dimensionality with a more limited number of interparticle bonds. It is not necessary to restrict the bonds to nearest-neighbor ones; additional bonds can readily be considered as long as their number remains small enough so that the sums of Δ functions are manageable. The two- and three-dimensional series, it will be observed, were obtained by the same algebraic technique as the one-dimensional one. Consequently, once a term in the one-dimensional series is known, the corresponding term for series in higher dimensions can be found without much additional effort. Since the technique is basically algebraic, it lends itself to programming by computer. It was pointed out that coefficients for the one-dimensional series were verified in this way. It may also prove feasible to determine expansion terms for series in higher dimensions by this method.

9. SUMMARY AND CONCLUSIONS

It was seen that the cell model underlying this study describes a simple one-dimensional fluid in which all particles interact with one another. The cells, as pointed out, serve only to specify the instantaneous position of the particles with an uncertainty equivalent to the particle dimension. Artificialities introduced by the model, in addition to this uncertainty in position, are the periodic boundary conditions and the hard-core repulsive potential that was assumed. The latter restricts cell occupancy to zero or one and hence causes the system to behave as an assembly of fermions. This permits an isomorphism to be established between cell occupation numbers and Ising spin states so that the Ising formalism can be applied to the model. In addition, the fermionlike nature of the system results in characteristic behavior, as evidenced by the primed sums and their expansion in the series formulation of the partition function and the commutation rules of the operators in Appendix B. This fermionlike behavior also underlies, of course, the success of the various operator methods and field-theoretical techniques that have been applied to the Ising model in recent years.[23-26]

We saw that in the present model the spinor-algebraic approach, which proved so successful in solving the two-dimensional Ising model, will not lead to a solution. The difficulty lies in the very much larger number of bonds per particle in our model. This results in an infinite coordination number in the thermodynamic limit. The operators of interest are therefore not the spin representatives of plane rotations but turn out to be parts of tensor transformations.

It proved possible, however, to diagonalize the operator, thus permitting the solution to be written as an infinite series. We saw that the series converges absolutely for all densities and offers a convenient method of examining the analyticity of the partition function. The results of this analysis agree with those of Yang and Lee.

In applying the solution to a one-dimensional system in which only nearest neighbors interact, we were able to verify the validity of the approach and develop a straightforward algebraic technique which proved very convenient for obtaining low-temperature series for two- and three-dimensional systems. These series were seen to agree with those obtained by other authors using entirely different methods. It is rather remarkable that the simple scheme of applying the potentials in Eqs. (2.12)–(2.14) will convert a one-dimensional system into one of higher dimension but with a reduced number of bonds per particle. Looked at from that point of view, the unsolved three-dimensional Ising model is really a subset of the more general one-dimensional system that forms the central problem of the present series of papers. If we can find a closed-form solution to the latter, then we have automatically solved the three-dimensional Ising model as well. The present analysis also sheds some interesting light on the reason why a two-dimensional array with nearest-neighbor and next-nearest-neighbor bonds should pose the same level of difficulty as the three-dimensional Ising problem. From Eqs. (2.13) and (2.14), we see that these two systems are mathematically completely isomorphic.

In the second of this series of two papers the solution will be applied to certain potentials for which the series can be summed in closed form. We shall see that for a system of point particles with no interaction potential the model correctly reproduces the equation of state of an ideal gas. If, on the other hand, we retain the repulsive core and consider a system of hard rods, we obtain the well-known Tonks equation of state. This solution will be seen to hold in one, two, and three dimensions. A one-dimensional fluid with only nearest-neighbor interactions is then examined briefly and is seen to have interesting thermodynamic properties but exhibits no phase transition, of course. If we let the range parameter in the

[23] H. S. Green and C. A. Hurst, *Order-Disorder Phenomena* (Interscience Publishers, New York, 1964).
[24] I. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).
[25] R. W. Gifford and R. A. Hurst, J. Math. Phys. **7**, 305 (1966); **8**, 1427 (1967).
[26] L. P. Kadanoff, Nuovo Cimento **44**, 276 (1966).

Lennard–Jones potential go to zero, we shall find that the system does experience a phase transition. The thermodynamic properties of this system are examined by computer for various volumes and are then examined analytically. In the thermodynamic limit the transition temperature goes to infinity so that a change of phase can occur at any finite temperature. Finally, finite systems of different sizes interacting with the unmodified potential are examined by computer. They are seen to exhibit very realistic thermodynamic behavior and give a number of indications of an incipient phase transitions. One of the most cogent of these is the behavior of the pair-correlation functions. There is obvious long-range order up to a certain temperature which coincides with the temperature at which the specific-heat curve has a maximum. For higher temperatures long-range order changes very rapidly to short-range order. Two- and three-dimensional systems with nearest-neighbor interactions are also examined numerically and are seen to have an incipient change of phase at temperatures that agree with those of the corresponding Ising model within quite close bounds.

APPENDIX A: PARTITION FUNCTIONS OF SMALL SYSTEMS

The following partition functions were computed directly from Eq. (3.5) of the text. All are written for a fluid, the symbols having the meaning defined in Sec. 2. To obtain the corresponding ferromagnetic partition function, it is only necessary to premultiply the expression given by the factor $\exp\{N(\Theta - \nu)\}$ and reinterpret the symbols as follows:

$$x_r = \exp\{8\theta_r\}, \qquad \theta_r = -\beta\phi_r,$$
$$\phi_r = \tfrac{1}{2}(J_r + J_{N-r}), \qquad \nu = \beta m B, \tag{A1}$$

where J_r is the exchange energy of two spins separated by r lattice spacings, m is the magnetic moment per spin, while B is the external magnetic field. Then we have

$$Q_2 = 2\exp(2\nu)\{\cosh(2\nu) + x_1^{-\frac{1}{2}}\}, \tag{A2}$$

$$Q_3 = 2\exp(3\nu)\{\cosh(3\nu) + 3x_1^{-1}\cosh(\nu)\}, \tag{A3}$$

$$Q_4 = 2\exp(4\nu)\{\cosh(4\nu) + 4x_1^{-1}x_2^{-\frac{1}{2}}\cosh(2\nu) + 2x_1^{-1}x_2^{-1} + x_1^{-2}\}, \tag{A4}$$

$$Q_5 = 2\exp(5\nu)\{\cosh(5\nu) + 5(x_1x_2)^{-1}\cosh(3\nu) + 5(x_1x_2)^{-2}(x_1 + x_2)\cosh(\nu)\}, \tag{A5}$$

$$Q_6 = 2\exp(6\nu)\{\cosh(6\nu) + 6(x_1x_2x_3^{\frac{1}{2}})^{-1}\cosh(4\nu) + 3(x_1x_2x_3^{\frac{1}{2}})^{-2}(2x_1 + 2x_2 + x_3)\cosh(2\nu) + (x_1x_2x_3^{\frac{1}{2}})^{-3}(6x_1x_2x_3 + 3x_1^2x_2 + x_2^3)\}, \tag{A6}$$

$$Q_7 = 2\exp(7\nu)\{\cosh(7\nu) + 7(x_1x_2x_3)^{-1}\cosh(5\nu) + 7(x_1x_2x_3)^{-2}(x_1 + x_2 + x_3)\cosh(3\nu) + 7(x_1x_2x_3)^{-3}(x_1^2x_2 + 2x_1x_2x_3 + x_1x_3^2 + x_2^2x_3)\cosh(\nu)\}, \tag{A7}$$

$$Q_8 = 2\exp(8\nu)\{\cosh(8\nu) + 8X^{-1}\cosh(6\nu) + 4X^{-2}(2x_1 + 2x_2 + 2x_3 + x_4)\cosh(4\nu) + 8X^{-3}(x_1^2x_2 + x_2^2x_4 + x_2x_3^2 + 2x_1x_2x_3 + 2x_1x_3x_4)\cosh(2\nu) + X^{-4}(4x_1^3x_2^2x_3 + 8x_1^2x_2^2x_3x_4 + 8x_1^2x_2x_3^2x_4 + 8x_1x_2^2x_3^2x_4 + 4x_1x_2^2x_3^3 + 2x_1^2x_3^2x_4^2 + x_2^4x_4^2)\}, \tag{A8}$$

where $X = x_1x_2x_3x_4^{\frac{1}{2}}$, and

$$Q_9 = 2\exp(9\nu)\{\cosh(9\nu) + 9X^{-1}\cosh(7\nu) + 9X^{-2}(x_1 + x_2 + x_3 + x_4)\cosh(5\nu) + 9X^{-3}(x_1^2x_2 + 2x_1x_2x_3 + 2x_1x_3x_4 + x_2^2x_4 + x_1x_4^2 + 2x_2x_3x_4 + \tfrac{1}{3}x_3^3)\cosh(3\nu) + 9X^{-4}(x_1^3x_2^2x_3 + 2x_1^2x_2^2x_3x_4 + x_1^2x_2x_3^2x_4 + 2x_1^2x_2x_3x_4^2 + 2x_1x_2^2x_3x_4^2 + x_1^2x_3x_4^3 + 2x_1x_2x_3^3x_4 + x_1x_2x_3^2x_4^2 + x_1x_2^2x_3^2x_4 + x_2^3x_3x_4^2)\cosh(\nu)\}, \tag{A9}$$

where $X = x_1x_2x_3x_4$.

APPENDIX B: SPINOR-ALGEBRAIC FORMULATION

Starting from Eq. (3.5) in the text, this appendix shows that the operator S is not the spin representative of a set of commuting plane rotations, but is part of a tensor transformation. Hence it does not appear feasible to determine its eigenvalues by the spinor-algebraic approach. In order to reduce the problem to its simplest terms, we shall consider only the case $\nu = 0$, i.e., $S_2 = 1$. We are then concerned with the operator

$$S_1 = \prod_{r=1}^{N}\prod_{s=1}^{N} D_{rs}, \quad \text{where} \quad D_{rs} = \exp\{Z_rZ_{r+s}\theta_s\}.$$

To proceed we define a set of matrices that are the generators of a complete set of linearly independent operators that span the space of the operator S and obey the following anticommutation rule:

$$[\Gamma_\alpha, \Gamma_\beta]_+ = 2\delta_{\alpha,\beta}. \tag{B1}$$

In the 2^N-dimensional representation that has been adopted for the Z_k [cf. Eq. (3.4)], the base matrices are the Γ matrices and all possible products of Γ matrices. It is readily shown that there are $2N$ independent

matrices of this type. We choose the following representation for the Γ's:

$$\Gamma_{2\alpha-1} = Z_1 \cdots Z_{\alpha-1} X_\alpha;\ \Gamma_{2\alpha} = Z_1 \cdots Z_{\alpha-1} Y_\alpha. \quad \text{(B2)}$$

We find then that the operator Z is given by

$$Z_\alpha = i\Gamma_{2\alpha}\Gamma_{2\alpha-1}, \quad \text{(B3)}$$

so that

$$\begin{aligned} D_{rs} &= \exp\{Z_r Z_{r+s}\theta_s\} \\ &= \exp\{-\theta_s \Gamma_{2r}\Gamma_{2r-1}\Gamma_{2(r+s)}\Gamma_{2(r+s)-1}\}. \end{aligned} \quad \text{(B4)}$$

Consider now the operator

$$D_{\mu\nu\rho\sigma} = \exp\{(\theta/2)\Gamma_\mu\Gamma_\nu\Gamma_\rho\Gamma_\sigma\}. \quad \text{(B5)}$$

One proves readily that

$$D_{\mu\nu\rho\sigma} = \cosh(\theta/2) + \Gamma_\mu\Gamma_\nu\Gamma_\rho\Gamma_\sigma \sinh(\theta/2), \quad \text{(B6)}$$

where the fact was used that $(\Gamma_\mu\Gamma_\nu\Gamma_\rho\Gamma_\sigma)^2 = 1$, provided that $\mu \neq \nu \neq \rho \neq \sigma$, which will be assumed in what follows. Let us first examine the properties of a related operator

$$G_{\mu\nu\rho\sigma} = \exp\{(\theta/2)(\Gamma_\mu\Gamma_\nu + \Gamma_\rho\Gamma_\sigma)\}. \quad \text{(B7)}$$

Observing that

$$(\Gamma_\mu\Gamma_\nu + \Gamma_\rho\Gamma_\sigma)^2 = 2(\Gamma_\mu\Gamma_\nu\Gamma_\rho\Gamma_\sigma - 1), \quad \text{(B8)}$$

we have

$$\begin{aligned} G_{\mu\nu\rho\sigma} &= \cos^2(\theta/2) + (\Gamma_\mu\Gamma_\nu + \Gamma_\rho\Gamma_\sigma)\sin(\theta/2) \\ &\quad \times \cos(\theta/2) + \Gamma_\mu\Gamma_\nu\Gamma_\rho\Gamma_\sigma \sin^2(\theta/2) \\ &= \tfrac{1}{2}\{S_{\mu\nu} + S_{\rho\sigma} + aD_{\mu\nu\rho\sigma} + b\}. \end{aligned} \quad \text{(B9)}$$

Here $\tanh\phi = 1 - \cos\theta$, $a = \operatorname{sech}\phi$, and b is related to a and ϕ by the equation

$$a^2 + b(b+2) = 0. \quad \text{(B10)}$$

The operator S in Eq. (B9) is defined as follows:

$$S_{\mu\nu}(2\theta) = \cos\theta + \Gamma_\mu\Gamma_\nu \sin\theta = \exp\{\theta\Gamma_\mu\Gamma_\nu\}. \quad \text{(B11)}$$

It is not difficult to show that this operator is the spin representative of a plane rotation in the $\mu - \nu$ plane through an angle 2θ.[3,8] We must now investigate the properties of the operator G. The analysis is simplified if we note that

$$[\Gamma_\mu\Gamma_\nu, \Gamma_\rho\Gamma_\sigma]_- = 0 \quad (\mu, \nu, \rho, \sigma \text{ distinct}), \quad \text{(B12)}$$

so that

$$\begin{aligned} G_{\mu\nu\rho\sigma} &= \exp\{(\theta/2)(\Gamma_\mu\Gamma_\nu + \Gamma_\rho\Gamma_\sigma) \\ &= \exp\{(\theta/2)\Gamma_\mu\Gamma_\nu\}\exp\{(\theta/2)\Gamma_\rho\Gamma_\sigma\} \\ &= S_{\mu\nu}(\theta)S_{\rho\sigma}(\theta) = S_{\rho\sigma}(\theta)S_{\mu\nu}(\theta). \end{aligned} \quad \text{(B13)}$$

It follows that $G^{-1}G = 1$ so that G is a unitary operator. One finds then that

$$\begin{aligned} \bar{\Gamma}_\mu\bar{\Gamma}_\nu &= G^{-1}\Gamma_\mu\Gamma_\nu G \\ &= \exp\{-(\theta/2)(\Gamma_\mu\Gamma_\nu + \Gamma_\rho\Gamma_\sigma)\}\Gamma_\mu\Gamma_\nu \\ &\quad \times \{\exp(\theta/2)(\Gamma_\mu\Gamma_\nu + \Gamma_\rho\Gamma_\sigma)\} \\ &= \Gamma_\mu\Gamma_\nu. \end{aligned} \quad \text{(B14)}$$

Similarly,

$$\begin{aligned} \bar{\Gamma}_\rho\bar{\Gamma}_\sigma &= G^{-1}\Gamma_\rho\Gamma_\sigma G = \Gamma_\rho\Gamma_\sigma, \\ \bar{\Gamma}_\alpha\bar{\Gamma}_\beta &= G^{-1}\Gamma_\alpha\Gamma_\beta G = \Gamma_\alpha\Gamma_\beta \quad (\alpha, \beta \neq \mu, \nu, \rho, \sigma). \end{aligned} \quad \text{(B15)}$$

But

$$\begin{aligned} \bar{\Gamma}_\mu\bar{\Gamma}_\rho &= G^{-1}\Gamma_\mu\Gamma_\rho G \\ &= \exp\{-(\theta/2)\Gamma_\mu\Gamma_\nu\}\Gamma_\mu \exp\{(\theta/2)\Gamma_\mu\Gamma_\nu\} \\ &\quad \times \exp\{-(\theta/2)\Gamma_\rho\Gamma_\sigma\}\Gamma_\rho \exp\{(\theta/2)\Gamma_\rho\Gamma_\sigma\} \\ &= (\Gamma_\mu\cos\theta + \Gamma_\nu\sin\theta)(\Gamma_\rho\cos\theta + \Gamma_\sigma\sin\theta) \\ &= \Gamma_\mu\Gamma_\rho\cos^2\theta + (\Gamma_\nu\Gamma_\rho + \Gamma_\mu\Gamma_\sigma)\sin\theta\cos\theta \\ &\quad + \Gamma_\nu\Gamma_\sigma\sin^2\theta. \end{aligned} \quad \text{(B16)}$$

And, similarly,

$$\begin{aligned} \bar{\Gamma}_\mu\bar{\Gamma}_\sigma = G^{-1}\Gamma_\mu\Gamma_\sigma G &= \Gamma_\mu\Gamma_\sigma\cos^2\theta + (\Gamma_\nu\Gamma_\sigma - \Gamma_\mu\Gamma_\rho) \\ &\quad \times \sin\theta\cos\theta - \Gamma_\nu\Gamma_\rho\sin^2\theta. \end{aligned} \quad \text{(B17)}$$

Other transformations follow the same pattern. Let us define a new vector X, whose $4N^2$ components are the second rank tensors $\Gamma_{\alpha\beta} = \Gamma_\alpha\Gamma_\beta$ ($\alpha, \beta = 1, 2, \cdots, 2N$). We can write these transformations symbolically as follows:

$$\bar{X} = \Omega X. \quad \text{(B18)}$$

The nonidentity elements of this transformation are

$$\begin{vmatrix} \bar{\Gamma}_\mu\bar{\Gamma}_\rho \\ \bar{\Gamma}_\mu\bar{\Gamma}_\sigma \\ \bar{\Gamma}_\nu\bar{\Gamma}_\rho \\ \bar{\Gamma}_\nu\bar{\Gamma}_\sigma \end{vmatrix} = \begin{vmatrix} \cos^2\theta & \sin\theta\cos\theta & \sin\theta\cos\theta & \sin^2\theta \\ -\sin\theta\cos\theta & \cos^2\theta & -\sin^2\theta & \sin\theta\cos\theta \\ -\sin\theta\cos\theta & -\sin^2\theta & \cos^2\theta & \sin\theta\cos\theta \\ \sin^2\theta & -\sin\theta\cos\theta & -\sin\theta\cos\theta & \cos^2\theta \end{vmatrix} \begin{vmatrix} \Gamma_\mu\Gamma_\rho \\ \Gamma_\mu\Gamma_\sigma \\ \Gamma_\nu\Gamma_\rho \\ \Gamma_\nu\Gamma_\sigma \end{vmatrix}. \quad \text{(B19)}$$

We note that

$$\Omega = \omega \otimes \omega \quad \text{(B20)}$$

and

$$X = \Gamma \otimes \Gamma,$$

where ω is a plane rotation with components

$$\begin{vmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{vmatrix} \quad \text{(B21)}$$

and Γ is a vector having the $2N$ Γ matrices as its components. Thus Ω is a tensor transformation transforming Γ dyadics into themselves. Using summation covention and covariant–contravariant notation, the transformation appears as follows:

$$\Gamma^{\mu\nu} = \Omega^{\mu\nu}_{\alpha\beta}\Gamma^{\alpha\beta}. \tag{B22}$$

It follows then that the operator G is the spin representative of a tensor transformation. D, on the other hand, is associated with the operator G through Eq. (B9) but is not itself a spin representative. Accordingly, it does not seem feasible to determine the eigenvalues of D by spinor-algebraic analysis.

APPENDIX C: CLOSED FORM SOLUTION FOR THE ONE-DIMENSIONAL MODEL WITH NEAREST-NEIGHBOR INTERACTIONS

We consider first the case $\nu = 0$. In that case Eq. (6.14) becomes

$$\begin{aligned} Q_N(\nu = 0) &= 2C_N\Big\{1 + N\sum_{n=1}^{[N/2]}\sum_{k=1}^{n}\frac{1}{k}\binom{n-1}{k-1} \\ &\quad\times\binom{N-n-1}{k-1}x_1^{-k}(1 - \tfrac{1}{2}\delta_{n,N/2})\Big\} \\ &= 2C_N\Big\{1 + N\sum_{k=1}^{[N/2]}\left(\frac{1}{2k}\right)x_1^{-k}\sum_{n=k}^{N-k}\binom{n-1}{k-1}\binom{N-n-1}{k-1}\Big\}, \end{aligned} \tag{C1}$$

where the order of summation was changed and the δ-function term was eliminated by taking advantage of the symmetry of the summand with respect to the substitution $n \to N - n$. If we now use the following relationship (which follows directly from the definition of the combinatorial symbol),

$$\binom{r-s}{t} = (-1)^t\binom{s-r+t-1}{t}, \tag{C2}$$

where for $a < 0$ we define

$$\binom{a}{b} = \frac{1}{b!}a(a-1)\cdots(a-b+1),$$

we find after some algebra that

$$\begin{aligned} \sum_{n=k}^{N-k}\binom{n-1}{k-1}\binom{N-n-1}{k-1} &= \sum_{n=k}^{N-k}(-1)^{N-2k}\binom{-k}{N-k-n}\binom{-k}{n-k} \\ &= \binom{N-1}{N-2k}. \end{aligned} \tag{C3}$$

The following identity was also used:

$$\sum_{r=0}^{k}\binom{m}{r}\binom{n}{k-r} = \binom{m+n}{k}. \tag{C4}$$

Thus for the partition function we have

$$\begin{aligned} Q_N(\nu = 0) &= 2C_N(\nu = 0)\Big\{1 + \sum_{k=1}^{[N/2]}\binom{N}{2k}x_1^{-k}\Big\} \\ &= C_N\sum_{k=0}^{N}\binom{N}{k}[1 + (-1)^k]x_1^{-k/2} \\ &= C_N\{(1 + x_1^{-\frac{1}{2}})^N + (1 - x_1^{-\frac{1}{2}})^N\} \\ &= 2^N C_N\exp(-N\epsilon)(\cosh^N\epsilon + \sinh^N\epsilon). \end{aligned} \tag{C5}$$

This agrees with the well-known solution of the one-dimensional Ising model in the absence of an external magnetic field.[3,15]

When $\nu \neq 0$, the analysis becomes considerably more complex. The closed-form solution of the one-dimensional Ising model is in that case (cf. Appendix D):

$$\begin{aligned} Q_N = C_N\cosh^N(\nu)\{&[1 + (1+\omega)^{\frac{1}{2}}]^N \\ &+ [1 - (1+\omega)^{\frac{1}{2}}]^N\}, \end{aligned} \tag{C6}$$

where $\omega = (x_1^{-1} - 1)\,\mathrm{sech}^2(\nu.)$ For the work to follow it is desirable to rewrite this by means of the binomial theorem in the form

$$\begin{aligned} Q_N = 2C_N\cosh^N(\nu)&\sum_{n=0}^{[N/2]}\sum_{k=0}^{n}\sum_{m=0}^{k}\binom{N}{2n}\binom{n}{k}\binom{k}{m} \\ &\times(-1)^{k-m}x_1^{-m}\cosh^{-2k}(\nu). \end{aligned} \tag{C7}$$

In order to show that Eq. (6.14) of the text leads to this expression, we must then establish the following equivalence:

$$\begin{aligned} &\cosh^N(\nu)\sum_{n=0}^{[N/2]}\sum_{k=0}^{n}\sum_{m=0}^{k}\binom{N}{2n}\binom{n}{k}\binom{k}{m} \\ &\quad\times(-1)^{k-m}x_1^{-m}\cosh^{-2k}(\nu) \\ &\quad\stackrel{?}{=}\cosh(N\nu) + \sum_{n=1}^{[N/2]}\sum_{k=1}^{n}\frac{N}{k}\binom{n-1}{k-1}\binom{N-n-1}{k-1}x_1^{-k} \\ &\quad\times\cosh[(N-2n)\nu](1 - \tfrac{1}{2}\delta_{n,N/2}). \end{aligned} \tag{C8}$$

For $m = 0$ we must show that

$$\begin{aligned} \cosh^N(\nu)\sum_{n=0}^{[N/2]}\sum_{k=0}^{n}\binom{N}{2n}\binom{n}{k}(-1)^k\cosh^{-2k}(\nu) \\ = \cosh(N\nu). \end{aligned} \tag{C9}$$

By retracing the steps that led from Eq. (C6) to (C7), we find that this proof is trivial. Suppose now that

Eq. (C8) holds for $m = m$; i.e., suppose that

$$\sum_{n=m}^{[N/2]}\sum_{k=m}^{n}\binom{N}{2n}\binom{n}{k}\binom{k}{m}(-1)^{k-m}\cosh^{-2k}(\nu)$$
$$=\binom{N}{m}\cosh^{-N}(\nu)\sum_{n=m}^{[N/2]}\binom{n-1}{m-1}\binom{N-n-1}{m-1}$$
$$\times\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}). \quad \text{(C10)}$$

We wish to show that it holds for $m = m + 1$, so that the equivalence of the following expression is to be proved:

$$\sum_{n=m}^{[N/2]}\sum_{k=m+1}^{n}\binom{N}{2n}\binom{n}{k}\binom{k}{m+1}(-1)^{k-m-1}\cosh^{-2k}(\nu)$$
$$\stackrel{?}{=}\binom{N}{m+1}\cosh^{-N}(\nu)\sum_{n=m+1}^{[N/2]}\binom{n-1}{m}\binom{N-n-1}{m}$$
$$\times\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}). \quad \text{(C11)}$$

This can be recast in the following more convenient way:

$$\cosh^{N}(\nu)\sum_{n=m}^{[N/2]}\sum_{k=m}^{n}\binom{N}{2n}\binom{n}{k}\binom{k}{m}$$
$$\times(k-m)(-1)^{k-m-1}\cosh^{-2k}(\nu)$$
$$=\frac{N}{m^2}\sum_{n=m}^{[N/2]}\binom{n-1}{m-1}\binom{N-n-1}{m-1}(n-m)(N-n-m)$$
$$\times\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}). \quad \text{(C12)}$$

We now let

$$F(N,\nu,m)$$
$$=\sum_{n=m}^{[N/2]}\sum_{k=m}^{n}\binom{N}{2n}\binom{n}{k}\binom{k}{m}(-1)^{k-m}\cosh^{-2k}(\nu). \quad \text{(C13)}$$

Then, using the assumed identity, Eq. (C10), the equivalence to be established is

$$\sum_{n=m}^{[N/2]}\sum_{k=m}^{n}\binom{N}{2n}\binom{n}{k}\binom{k}{m}(k-m)(-1)^{k-m-1}\cosh^{-2k}(\nu)$$
$$=\tfrac{1}{2}(\coth\nu\,\partial/\partial\nu+2m)\Big[\frac{N}{m}\operatorname{sech}^{N}(\nu)$$
$$\times\sum_{n=m}^{[N/2]}\binom{n-1}{m-1}\binom{N-n-1}{m-1}$$
$$\times\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2})\Big]$$
$$=(N/2m)\operatorname{sech}^{N}(\nu)\sum_{n=m}^{[N/2]}\binom{n-1}{m-1}\binom{N-n-1}{m-1}$$
$$\times\{(N-2n)\coth(\nu)\sinh[(N-2n)\nu]$$
$$+(2m-N)\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}). \quad \text{(C14)}$$

This last equation can be re-expressed as follows:

$$\sum_{n=m}^{[N/2]}\sum_{k=m}^{n}\binom{N}{2n}\binom{n}{k}\binom{k}{m}(k-m)(-1)^{k-m-1}\cosh^{-2k}(\nu)$$
$$=(N/m)\operatorname{sech}^{N}(\nu)$$
$$\times\sum_{n=m+1}^{[N/2]}\Big\{\sum_{k=m+1}^{n}\binom{k-2}{m-1}\binom{N-k}{m-1}(N-2k+2)$$
$$-\binom{n-1}{m-1}\binom{N-n-1}{m-1}(n-m)\Big\}$$
$$\times\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}), \quad \text{(C15)}$$

where the following identities were used (which are readily established):

$$\coth(\nu)\sinh[(N-2n)\nu]$$
$$=\begin{cases}0 & (n=N/2),\\ \cosh[(N-2n)\nu] & \\ \quad+2\sum_{k=1}^{[N/2]-n}\cosh[(N-2n-2k)\nu] & \\ \quad\times(1-\tfrac{1}{2}\delta_{k,[N/2]-n}) & (n\neq N/2),\end{cases} \quad \text{(C16)}$$

and

$$\sum_{n=m}^{[N/2]}\sum_{k=1}^{[N/2]-n}\binom{n-1}{m-1}\binom{N-n-1}{m-1}(N-2n)$$
$$\times\cosh[(N-2n-2k)\nu]$$
$$\times(1-\tfrac{1}{2}\delta_{k,[N/2]-n})(1-\delta_{n,N/2})$$
$$=\sum_{n=m+1}^{[N/2]}\sum_{k=m+1}^{m}\binom{k-2}{m-1}\binom{N-k}{m-1}(N-2k-2)$$
$$\times\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}). \quad \text{(C17)}$$

To complete the proof by induction, one must show [cf. Eq. (C12)] that

$$(N/m)\sum_{n=m+1}^{[N/2]}\sum_{k=m+1}^{n}\Big\{\binom{k-2}{m-1}\binom{N-k}{m-1}(N-2k+2)$$
$$-\binom{n-1}{m-1}\binom{N-n-1}{m-1}(n-m)\Big\}$$
$$\times\cosh(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2})$$
$$=(N/m^2)\sum_{n=m}^{[N/2]}\binom{n-1}{m-1}\binom{N-n-1}{m-1}(n-m)$$
$$\times(N-n-m)\cosh[(N-2n)\nu](1-\tfrac{1}{2}\delta_{n,N/2}). \quad \text{(C18)}$$

Recognizing that ν is arbitrary, this is equivalent to

establishing the following identity:

$$\sum_{k=m+1}^{n}\left\{\binom{k-2}{m-1}\binom{N-k+1}{m}-\binom{k-1}{m}\binom{N-k}{m-1}\right\}=\binom{n-1}{m}\binom{N-n}{m}. \quad \text{(C19)}$$

For $m = 1$ the proof is trivial. The identity is readily established in general if one expands the left-hand side of (C19) as

$$\begin{aligned}&\binom{m-1}{m-1}\binom{N-m}{m}-\binom{m}{m}\binom{N-m-1}{m-1}\\&\quad+\binom{m}{m-1}\binom{N-m-1}{m}\\&\quad-\binom{m+1}{m}\binom{N-m-2}{m-1}+\cdots\\&\quad+\binom{n-2}{m-1}\binom{N-n+1}{m}-\binom{n-1}{m}\binom{N-n}{m-1}\end{aligned} \quad \text{(C20)}$$

and uses the following two relations:

$$\binom{r}{s}-\binom{r-1}{s-1}=\binom{r-1}{s}, \quad \text{(C21)}$$

$$\binom{r}{s}+\binom{r}{s-1}=\binom{r+1}{s}. \quad \text{(C22)}$$

This completes the inductive proof of the equivalence of Eq. (6.14) and (C6).

APPENDIX D: CLOSED FORM SOLUTION OF THE ONE-DIMENSIONAL SYSTEM WITH NEAREST-NEIGHBOR INTERACTIONS

From Eq. (2.10) using the potential of Eq. (6.1), we obtain

$$\begin{aligned}Q_N&=A_N\sum_{\{\sigma\}}\exp\left\{\epsilon\sum_{r=1}^{N}\sigma_r\sigma_{r+1}+\nu\sum_{r=1}^{N}\sigma_r\right\}\\&=A_N\sum_{\{\sigma\}}\langle\sigma_1|\,P\,|\sigma_2\rangle\langle\sigma_2|\,P\,|\sigma_3\rangle\cdots\langle\sigma_N|\,P\,|\sigma_1\rangle\\&=A_N T_r\{P^N\}=A_N(\lambda_+^N+\lambda_-^N),\end{aligned} \quad \text{(D1)}$$

where

$$P=\begin{vmatrix}e^{\epsilon+\nu} & e^{-\epsilon}\\ e^{-\epsilon} & e^{\epsilon-\nu}\end{vmatrix} \quad \text{(D2)}$$

and λ_+ and λ_- are the eigenvalues of P. We find readily that

$$\lambda_\pm=\exp(\epsilon)\{\cosh\nu\pm[\cosh^2\nu-2\exp(-2\epsilon)\sinh(2\epsilon)]^{\frac{1}{2}}\}. \quad \text{(D3)}$$

Hence

$$Q_N=A_N\exp(N\epsilon)\cosh^N(\nu)\{[1+(1+\omega)^{\frac{1}{2}}]^N+[1-(1+\omega)^{\frac{1}{2}}]^N\}, \quad \text{(D4)}$$

where $\omega=(x_1^{-1}-1)\operatorname{sech}^2(\nu)$ and $x_1=\exp(4\epsilon)$. And since

$$A_N=\begin{cases}N(\nu-\epsilon) & \text{(fluid)},\\ 1 & \text{(ferromagnet)},\end{cases} \quad \text{(D5)}$$

we obtain

$$Q_N=C_N\cosh^N(\nu)\{[1+(1+\omega)^{\frac{1}{2}}]^N+[1-(1+\omega)^{\frac{1}{2}}]^N\}, \quad \text{(D6)}$$

where

$$C_N=\begin{cases}\exp(N\nu) & \text{(fluid)},\\ \exp(N\epsilon) & \text{(ferromagnet)}.\end{cases} \quad \text{(D7)}$$