Treatment of the exchange-interaction model by means of the symmetric group

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The representation theory of the symmetric group is used to study the spin-S exchange-interaction model of ferromagnetism within the infinite-range approximation. The $2S$ order parameters are determined by the row lengths of the Young diagram that specifies the free-energy extrema. The set of solutions of the order-parameter equations has been fully explored. Stability analysis shows that one of the solutions represents the absolute minimum and describes the thermodynamically stable state. This solution coincides with the mean-field solution due to Chen *et al.* [Phys. Rev. B **46**, 8323 (1992)]. The other nontrivial solutions correspond to saddle points in the free-energy surface, with consecutively increasing indices.

I. INTRODUCTION

The exchange-interaction model is defined by the many-body Hamiltonian

$$H=-J\sum_{\langle ij\rangle} P_{ij}\,, \tag{1}$$

in which P_{ij} is the transposition of the indices i and j and $\langle ij\rangle$ stands for a nearest-neighbor pair. A mean-field treatment of this Hamiltonian was proposed by Chen, Gou, and Chen.[1] That treatment, as well as several other treatments of the same Hamiltonian,[2–7] is based on the representation of the transpositions in terms of spin operators, in a manner that for spin-$\frac{1}{2}$ particles was proposed by Dirac,[8] and for particles of higher spin was developed by Schrödinger.[9] This representation shows that for spin $\frac{1}{2}$ the exchange-interaction model coincides with the Heisenberg Hamiltonian, whereas for higher spins it corresponds to the introduction of terms involving higher powers of $(\mathbf{S}_i\cdot\mathbf{S}_j)$. Thus, for a system of particles with elementary spin S, Chen *et al.*[1] introduce a set of $4S(S+1)$ order parameters which are the averages of the components of appropriate spin tensor operators. On the basis of reasonable indications that include an earlier treatment of the spin-1 case,[2] they conjecture these order parameters to have a common temperature dependence. The principal result of the mean-field approximation is that for $S>\frac{1}{2}$ the system exhibits a single first-order phase transition. This conclusion is supported by more sophisticated treatments.[3,7]

In the present paper we investigate the infinite-range counterpart of the exchange-interaction model. In several related contexts the equivalence of the mean-field and infinite-range treatments had been established. The infinite-range approach involves a well-defined approximation of the Hamiltonian, which is then solved exactly. The order parameters are uniquely determined as thermal averages of the quantum numbers that specify the energies and degeneracies of the Hamiltonian. This approach enables the treatment of Hamiltonians that involve an arbitrarily complicated dependence on the order parameters, in a manner that was explored for higher-order spin Hamiltonians.[10,11] Furthermore, it allows the construction of the full free-energy surface, which is needed for the study of time-dependent phenomena[12] and nonequilibrium properties.

Within the presently proposed treatment of the exchange-interaction model, there is no need to express the Hamiltonian in terms of spin operators. The eigenvalues and degeneracies are shown to be related to the characters and dimensions of the irreducible representations of the symmetric group (Sec. II A). The relevant quantum numbers are the row lengths of the Young diagrams that specify these representations, and the order parameters are the corresponding thermal averages. The maximal number of rows in the allowed Young diagrams is determined by the value of the elementary spin. The equations satisfied by the $2S$ order parameters are derived in Sec. II B and solved in Sec. III A. All the order parameters bifurcate from the trivial solution at a common temperature, which is a highly degenerate extremum of the free energy. A stability analysis shows that one of the solutions, which coincides with the mean-field solution obtained by Chen *et al.*,[1] represents the thermodynamically stable ordered state (Sec. III B). The other solutions are saddle points with well-defined indices on the free-energy surface.

II. STATISTICAL MECHANICS OF THE INFINITE-RANGE EXCHANGE MODEL

A. Group-theoretical preliminaries

The infinite-range exchange-interaction Hamiltonian is

$$H=-\frac{J}{N}\sum_{i<j}^{N} P_{ij}\,, \tag{2}$$

where N is the number of spins. The operator $\Sigma_{i<j}^{N}P_{ij}$ consists of all the transpositions of two indices, which form a conjugacy class of the symmetric group S_N. Its eigenvalues are (up to a normalization factor) equal to the corresponding irreducible characters. The latter are specified by means of Young diagrams $\Gamma\equiv\{\mu_1,\mu_2,\dots\}$, where $\mu_1\geqslant\mu_2\geqslant\cdots$ and $\mu_1+\mu_2+\cdots=N$. Particles with an elementary spin S give rise to irreducible representations whose Young diagrams contain at most $n=2S+1$ rows. The eigenvalues of

the transposition conjugacy class sum corresponding to Young diagrams with at most n rows are given by[13]

$$\Lambda_\Gamma = \frac{1}{2}\sum_{i=1}^{n} \mu_i(\mu_i - 2i). \tag{3}$$

The dimension of the irreducible representation Γ is

$$\Omega_\Gamma = N!\frac{\prod_{i<j}^{n}(\mu_i-\mu_j+j-i)}{\prod_{i=1}^{n}(\mu_i+n-i)!}. \tag{4}$$

N identical particles with an elementary spin S give rise to a total of $(2S+1)^N$ states. The irreducible representation Γ appears in the space spanned by these states

$$g_S(N,\Gamma) = \frac{\prod_{i<j}^{n}(\mu_i-\mu_j+j-i)}{\prod_{i<j}^{n}(j-i)}$$

times. Thus, $\Sigma_\Gamma g_S(N,\Gamma)\Omega_\Gamma = (2S+1)^N$.

B. The order-parameter equations

It will be convenient to introduce the reduced row lengths $\lambda_i = \mu_i/N$, which satisfy $\Sigma_{i=1}^n \lambda_i = 1$. In the thermodynamic limit the energy per particle obtains the form

$$e_\Gamma = -\frac{J}{2}\sum_{i=1}^{n}\lambda_i^2. \tag{5}$$

The number of states having this energy is $g_S(N,\Gamma)\Omega_\Gamma$. In the thermodynamic limit the entropy per particle becomes

$$s_\Gamma = -k\sum_{i=1}^{n}\lambda_i \ln(\lambda_i). \tag{6}$$

The reduced row lengths serve as the order parameters. Differentiating the free energy per particle

$$a_\Gamma = -\frac{J}{2}\sum_{i=1}^{n}\lambda_i^2 + kT\sum_{i=1}^{n}\lambda_i\ln(\lambda_i) \tag{7}$$

with respect to λ_m, we obtain

$$\lambda_m = \frac{1}{q}\exp(\beta J\lambda_m), \quad m=1,2,\ldots,n, \tag{8}$$

where $q=\Sigma_{i=1}^n \exp(\beta J\lambda_i)$. Equation (8) implies that $\exp(\beta J\lambda_1)/\lambda_1 = \exp(\beta J\lambda_2)/\lambda_2 = \cdots = \exp(\beta J\lambda_n)/\lambda_n$. Since the function $\exp(x)/x$, $x>0$, has a single minimum, it follows that the n-order parameters $\lambda_1, \lambda_2, \ldots, \lambda_n$ can have at most two different values. Since these order parameters are the row lengths of a Young diagram, they must satisfy $\lambda_1 = \lambda_2 = \cdots = \lambda_m \equiv \lambda_-$ and $\lambda_{m+1} = \lambda_{m+2} = \cdots = \lambda_n \equiv \lambda_+$, where $\lambda_- \geqslant \lambda_+$ [and $m\lambda_- + (n-m)\lambda_+ = 1$]. Here, m can obtain any of the values $1,2,\ldots,n-1$. The mth solution is specified by the single order parameter $\delta_m = \lambda_- - \lambda_+$ that satisfies the consistency equation

$$\delta_m = \frac{\exp(\beta J\delta_m)-1}{m\exp(\beta J\delta_m)+(n-m)}. \tag{9}$$

III. THE PHASE DIAGRAM

A. Solution of the order-parameter equations

We note that the trivial solution $\delta_m = 0$ always exists. This solution describes the ''isotropic'' phase, for which $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1/n$.

The consistency equation for δ_1 coincides with the mean-field equation derived by Chen *et al.*[1] For $S>\frac{1}{2}$ it yields a first-order transition. To investigate the whole set of solutions we find it convenient to write the consistency equation, Eq. (9), in the inverted form

$$kT = \frac{J\delta_m}{\ln\left(\frac{1+(n-m)\delta_m}{1-m\delta}\right)}. \tag{10}$$

Expanding the right-hand side for $\delta_m \to 0$ we obtain $\delta_m \simeq 2(T-T_0)/T(n-2m)$, where $kT_0 = J/n$. Thus, all the equations have a common temperature T_0 at which the nontrivial solution bifurcates from the trivial solution. For $m<n/2$ the δ_m vs T curve bifurcates towards higher temperatures, exhibiting a first-order-like behavior. For $m>n/2$, the curve of δ_m vs T exhibits a monotonic rise upon lowering the temperature. For even n (half-odd S) $\delta_{n/2}$ exhibits a critical behavior, satisfying the mean-field equation $\delta' = \frac{1}{2}\tanh(\beta J'\delta')$, where $J' = 2J/n$ and $\delta' = n\delta/4$.

Inspecting the expression for the energy, Eq. (5), we note that in the limit $T\to 0, \lambda_+ \to 0$ and $\lambda_- \to 1/m$ (since $\Sigma_{i=1}^n \lambda_i = 1$). Hence, the low-temperature limit of δ_m is $1/m$.

We now obtain the temperatures of the first-order transitions of the solutions $\delta_m>0$, $m<n/2$. From the equations $m\lambda_- + (n-m)\lambda_+ = 1$ and $\lambda_- - \lambda_+ = \delta_m$ we obtain $\lambda_- = [1+(n-m)\delta_m]/n$ and $\lambda_+ = (1-m\delta_m)/n$. Equating the free-energy per particle for the solution $\delta_m>0$ with that for the isotropic solution and using Eq. (10) to eliminate the temperature, we obtain

$$(n-m)\left(1-\frac{m\delta_m}{2}\right)\ln\left(\frac{1}{1-m\delta_m}\right) = m\left(1+\frac{(n-m)\delta_m}{2}\right)\ln[1+(n-m)\delta_m].$$

The expression presented was written in such a way that both prelogarithmic coefficients and both logarithms are positive. This transcendental equation happens to have a simple analytic solution, for which both the prelogarithmic coefficients and the arguments of the logarithmic functions are equal to one another. Equating either the former or the latter pair, we obtain

$$\delta_m^c = \frac{n-2m}{m(n-m)}.$$

The temperature at which the isotropic and $\delta_m>0$ free energies equalize can be obtained from Eq. (10), which yields

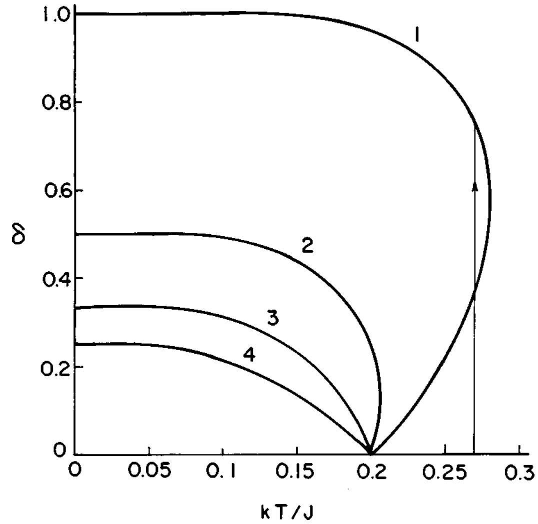

FIG. 1. Temperature dependence of the various order parameters for $S=2$. The vertical arrow specifies the first, order phase transition.

$$T_c(m)=J\frac{n-2m}{2m(n-m)\ln\left(\frac{n-m}{m}\right)}.$$

For $m=1$ these expressions coincide with those obtained by Chen *et al.*[1] From the expression for the critical temperature we note that the latter is a decreasing function of m, which means that the highest temperature transition from the isotropic phase is the transition into the state $\delta_1>0$. For the spin S Heisenberg Hamiltonian the classical limit $S\to\infty$ yields the Langevin instead of the Brillouin function in the order-parameter equation. We take $n\to\infty$ to mean the classical limit in the exchange-interaction model, and note that in this limit $T_c\to 0$, which suggests that this model is ''strictly quantum mechanical,'' possessing no classical limit.

The solutions of these equations for a system of particles with elementary spins $S=2$ are presented in Fig. 1.

B. Thermodynamic significance of the different solutions

To elucidate the nature of the different solutions, one needs to examine the structure of the free-energy surface, given by Eq. (7). Since all the solutions are free-energy extrema, their precise character is determined by the index of the Hessian matrix. The latter is obtained by differentiating the free energy twice with respect to the n (dependent) order parameters $\lambda_1,\lambda_2,\ldots,\lambda_n$, Eq. (7), obtaining $\partial^2 a/\partial\lambda_m^2=-J+(kT/\lambda_m)\equiv\alpha_m$. Denoting the variations in the order parameters by $x_1,x_2,\ldots,x_n$ and recalling the condition $\lambda_1+\lambda_2+\cdots+\lambda_n=1$ that implies $x_1+x_2+\cdots+x_n=0$, we obtain, in terms of the $(n-1)$-independent variations $x_1,x_2,\ldots,x_{n-1}$, the quadratic form

$$\delta a=\sum_{i=1}^{n-1}(\alpha_i+\alpha_n)x_i^2+2\alpha_n\sum_{i<j}^{n-1}x_ix_j.$$

The corresponding Hessian matrix is

$$\begin{pmatrix} \alpha_1+\alpha_n & \alpha_n & \alpha_n & \cdots & \alpha_n \\ \alpha_n & \alpha_2+\alpha_n & \alpha_n & \cdots & \alpha_n \\ \alpha_n & \alpha_n & \alpha_3+\alpha_n & \cdots & \alpha_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha_n & \alpha_n & \alpha_n & \cdots & \alpha_{n-1}+\alpha_n \end{pmatrix}. \quad (11)$$

At this stage it will be convenient to denote α_n by α_0. The determinant of the rth principal minor of the Hessian matrix is easily shown to be

$$\det{}_r=\left(\prod_{i=0}^{r}\alpha_i\right)\sum_{j=0}^{r}\frac{1}{\alpha_j}.$$

For the isotropic solution $\lambda_i=1/n$, hence $\alpha_i=-J+nkT=nk(T-T_0)$. The determinant of the rth minor of the Hessian matrix becomes $(r+1)[nk(T-T_0)]^r$, which is positive for all r when $T>T_0$, and which alternates in sign, beginning with a negative sign for the lowest minor, when $T<T_0$. It was already established that the isotropic solution is the absolute minimum for $T>T_c(1)$. In view of the present stability analysis it follows that this solution is a local minimum within the temperature range $T_0<T<T_c(1)$ and a maximum below T_0.

For the mth solution $(\delta_m>0)\,\alpha_1=\alpha_2=\cdots=\alpha_m\equiv\alpha_-=-J+(kT/\lambda_-)$ and $\alpha_{m+1}=\alpha_{m+2}=\cdots=\alpha_n\equiv\alpha_+=-J+(kT/\lambda_+)$. In this case the determinants of the first m principal minors are given by $\alpha_+\alpha_-^r(1/\alpha_++r/\alpha_-)$; $r=1,2,\ldots,m$ and those of the following minors are $\alpha_-^m\alpha_+^{r+1-m}[m/\alpha_-+(r+1-m)/\alpha_+]$; $r=m+1,m+2,\ldots,n-1$. In particular, the determinant of the complete Hessian matrix becomes

$$\alpha_-^{m-1}\alpha_+^{n-m-1}\left(-nJ+\frac{kT}{\lambda_-\lambda_+}\right).$$

For $T\to 0$, $\lambda_-\to 1/m$ and $\lambda_+\to 0$. Hence, in this limit $\alpha_-=-J$ and α_+ is positive and very large. Therefore, the first m minors alternate in sign, beginning with a positive sign for the lowest minor, but the remaining minors have a constant sign. Thus, this solution is a saddle point of index $m-1$ (the number of sign alternations of the sequence of determinants of the principal minors). In particular, the solution $\delta_1>0$ is a (local) minimum. For the solutions $\delta_m>0, m<\lfloor n/2\rfloor$, the ''spinodal'' point, at which the order-parameter curves backwards, can be determined by solving $\partial T/\partial\delta_m=0$ along with the order-parameter equation, Eq. (10). One obtains $nJ=kT/\lambda_-\lambda_+$. Comparing with the expression for the determinant of the Hessian matrix, we note that the latter vanishes at the ''spinodal point,'' allowing the index of the Hessian matrix to increase by unity at the lower branch of the order-parameter curve relative to the higher branch. The value of the order parameter at the ''spinodal point'' satisfies $\ln(\lambda_-/\lambda_+)=1/n(1/\lambda_+-1/\lambda_-)$ [along with $m\lambda_-+(n-m)\lambda_+=1$].

In conclusion, the system exhibits only two thermodynamically stable phases. For temperatures higher than $T_c(1)$, the absolute minimum corresponds to the isotropic phase, and below that temperature the phase $\delta_1>0$ has the lowest free energy. The free-energy surface exhibits a complex temperature dependence. Above the highest spinodal temperature it has a single (isotropic) minimum. Between that temperature and the highly degenerate bifurcation temperature T_0 it develops a rich manifold of extrema that corresponds to the solutions $\delta_m > 0$, $m < n/2$. Finally, at T_0 a further set of extrema emerges, corresponding to $n/2 \leq m \leq n$.

The connection between the order parameter δ_1 and the total spin of the system requires some consideration. For spin-$\frac{1}{2}$ particles $(n=2)$, each Young diagram corresponds to a well-defined total spin, $S_t = (\lambda_1 - \lambda_2)/2$. Thus, in this case δ_1 specifies the temperature dependence of the magnetization. The situation becomes more involved for higher elementary spins, since in these cases each Young diagram corresponds to a set of different total spins, with different weights. The solution $\delta_1 > 0$ specifies a Young diagram that represents a closed shell plus $N' = N\delta_1$ particles in a permutationally symmetric state (single-row Young diagram). One can show that when the elementary spin is $S=1$, a single-row Young diagram of length N' gives rise to all the total spin states $S_t = N', N'-2, N'-4, \ldots, 0$ or 1, each with weight 1. The average of these total spins (taking into account their multiplicities $2S_t+1$) is easily calculated, and in the thermodynamic limit (large N) is equal to $\frac{2}{3}N\delta_1$.

IV. CONCLUSIONS

The exchange-interaction model was investigated in the infinite-range limit. The significance of the Hamiltonian within the symmetric group was used to obtain both the energy and the degeneracy in terms of the representation theory of the latter. This approach avoids the transformation of the Hamiltonian into a polynomial in spin-tensor operators. For a system consisting of particles with an elementary spin S, the total number of order parameters is equal to $2S$. The $4S(S+1)$ order parameters introduced by Chen *el al.*[1] are the components of $2S$ irreducible tensor operators of ranks $l = 1, 2, \ldots, 2S$, the dynamical content of each one of which is, according to the Wigner-Eckart theorem, fully specified by a single reduced matrix element. The present treatment allowed the investigation of all the solutions of the coupled mean-field equations without any prior assumptions. In fact, it was established that the different order parameters are fully decoupled in the sense that only solutions in which at most one order parameter is nonvanishing are possible. The solution corresponding to the lowest free energy coincides with that given by Chen *et al.*,[1] exhibiting a first-order transition. The other solutions correspond to saddle points of different indices in the free-energy vs order-parameter space. The lowest $\lfloor S \rfloor$ solutions exhibit a first-order-like temperature dependence. In spite of the fact that all of these solutions but the lowest do not correspond to thermodynamically stable phases, they may well play a significant role in the nonequilibrium kinetics of the phase transitions.

The generalization to Hamiltonians involving exchange of several particles is one direction to which the present approach can be easily applied. This is a consequence of the fact that the degeneracy is not affected by such a modification of the Hamiltonian (as long as the infinite-range limit is considered), and the energy is given in terms of the eigenvalues of the higher single-cycle conjugacy class sums of the symmetric group. These eigenvalues are well-known polynomials in the row lengths of the Young diagrams, which in this context serve as the order parameters. It is very likely that such generalized Hamiltonians can give rise to more complex phase diagrams, which may involve chains of phase transitions between different ordered phases and possibly reentrant behavior.

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[1] H.H. Chen, S.C. Gou, and Y.C. Chen, Phys. Rev. B **46**, 8323 (1992).
[2] H.H. Chen and P.M. Levy, Phys. Rev. B **7**, 4267 (1973).
[3] H.A. Brown, Phys. Rev. B **31**, 3118 (1985); **40**, 775 (1989).
[4] H.H. Chen and F. Lee, Phys. Rev. B **42**, 10 540 (1990); **48**, 9456 (1993).
[5] S.C. Gou and H.H. Chen, Phys. Rev. B **49**, 1450 (1994).
[6] Y.M. Kao, F. Lee, and H.H. Chen, Phys. Rev. B **53**, 8192 (1996).
[7] Y.C. Chen, Phys. Rev. B **57**, 5009 (1998).
[8] P.A.M. Dirac, Proc. R. Soc. London, Ser. A **123**, 714 (1929).
[9] E. Schroedinger, Proc. R. Ir. Acad. Sect. A, Math. Astron. Phys. Sci. **47**, 39 (1941).
[10] J. Katriel and G.F. Kventsel, Phys. Rev. A **28**, 3037 (1983); Solid State Commun. **52**, 689 (1984); Phys. Rev. B **30**, 2828 (1984); **33**, 6360 (1986).
[11] Z. Pawlowska, J. Oliker, G.F. Kventsel, and J. Katriel, Phys. Rev. B **39**, 7140 (1989).
[12] G.F. Kventsel and J. Katriel, Phys. Rev. B **31**, 1559 (1985).
[13] I. G. Macdonald, *Symmetric Functions and Hall Polynomials*, 2nd ed. (Clarendon Press, Oxford, 1995).