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Solvable Compressible Ising Model

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The results for the solvable Baker–Essam model of a compressible Ising lattice are rederived by utilizing the equivalence of the system to a set of linear chains each described by the Mattis–Schultz one-dimensional magnetostriction model.

The long-standing controversial question as to the effects of lattice compressibility on magnetic phase transitions has attracted especially wide interest in the last two years following the publication of a paper by Baker and Essam[1] (BE). These authors displayed an exactly solvable model of a compressible harmonic lattice of spins interacting via a spatially dependent ferromagnetic Ising coupling. They found that when the system is constrained to constant volume or constant positive pressure the magnetic phase transition is second order with renormalized[2] critical exponents. Subsequently, Gunther, Bergman, and Imry[3] (GBI) showed that when this system is constrained to constant negative pressure the system undergoes a first-order transition.

In view of the wide interest in this subject it is worthwhile to display an alternate derivation of the results for the BE model which is considerably more transparent both physically and algebraically. BE evaluate the partition function directly, treating the lattice vibrations classically and constraining the surface atoms to their appropriate crystal faces. By contrast, I first transform the model Hamiltonian to describe two independent systems. The first system is a set of independent harmonic linear chains and the second is a three-dimensional Ising system of *rigid* spins interacting via an effective exchange coupling. Evaluation of the partition function then follows trivially. The transformed Hamiltonian is obtained utilizing the equivalence of the BE model to a set of linear chains, each described by the one-dimensional magnetostriction model of Mattis and Schultz.[4] A canonical transformation removes the spin-phonon interaction terms for each linear chain. In contrast to BE, the lattice vibrations are treated quantum mechanically and terms are included in the Hamiltonian to describe the action of a constant and equal compressional or tensile force applied to each surface atom, rather than to constrain these atoms to their crystal faces.

The BE model is characterized by the following three features: (i) The crystal lattice is simple cubic (lattice spacing a); (ii) the interatomic potential links nearest neighbors only and is chosen as $V_{ij}=V(a)+\hat{e}_{ij}\cdot(\vec{u}_i-\vec{u}_j)V'(a)+\frac{1}{2}[\hat{e}_{ij}\cdot(\vec{u}_i-\vec{u}_j)]^2V''$, where $\vec{u}_i$, $\vec{u}_j$ denote the vector displacements of the nearest-neighbor atoms i, j from their thermal equilibrium positions, $\hat{e}_{ij}$ is a unit vector pointing from the equilibrium position of j to i, and V'' is a constant independent of a. The shear-term quadratic in atomic displacements $V'(a)[\hat{e}_{ij}\times(\vec{u}_i-\vec{u}_j)]^2/2a$ of a central interatomic potential is specifically excluded by BE. (iii) The Ising spin interaction links nearest neighbors only, and its spatial dependence is chosen as $J_{ij}=J(a)+\hat{e}_{ij}\cdot(\vec{u}_i-\vec{u}_j)J'$, where J' is a constant.

It is convenient to take the crystal as a cube of N^3 atoms whereby each surface atom is subjected to a constant and equal compressional or tensile force applied normal to the crystal faces. Thus we add to the Hamiltonian[5] a term, $-F\vec{u}_s\cdot\hat{n}$, for each atom s lying in a crystal face characterized by the unit vector $\hat{n}$, the outwardly directed normal to that face. Positive (negative) values of the force $F\hat{n}$ on the surface atom correspond to tension (compression). For the simple cubic lattice, one has the identity $-F\sum_{\hat{n}s}\vec{u}_s\cdot\hat{n}=-F\sum_{\langle i,j\rangle}(\vec{u}_i-\vec{u}_j)\cdot\hat{e}_{ij}$, where $\langle i, j\rangle$ means that the summation includes all distinct nearest-neighbor pairs of atoms comprising the crystal. Including the above term leads to the model Hamiltonian

$$H=3N^3V(a)+H_I+\sum_i\frac{p_i^2}{2M}+\sum_{\langle i,j\rangle}\{[V'(a)-F-J'\sigma_i\sigma_j]\hat{e}_{ij}\cdot(\vec{u}_i-\vec{u}_j)+\tfrac{1}{2}V''[\hat{e}_{ij}\cdot(\vec{u}_i-\vec{u}_j)]^2\},\tag{1}$$

where

$$H_I = -\,J(a) \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

is the Ising Hamiltonian for spins situated on the rigid version of the lattice. For the simple cubic lattice the equilibrium sites can be imagined as defining a grid of three sets of mutually perpendicular rows lying parallel to the edges of the cube. Three intersecting cube edges are chosen as x, y, and z axes. Thus, the three sets of rows are parallel to these axes and they will be referred to as x, y, and z rows, respectively. Note that each lattice site is situated at the intersection of an x, a y, and a z row. It is then easy to show that $H - 3N^3V(a) - H_I$ reduces to a sum of $3N^2$ one-dimensional row Hamiltonians each of the form

$$\mathcal{H} = \sum_{n=1}^{N-1} \left(\frac{p_n^2}{2M} + (V' - F - J'\sigma_n\sigma_{n+1})(u_{n+1} - u_n) + \frac{1}{2} V''(u_{n+1} - u_n)^2 \right) + \frac{p_N^2}{2M} \quad . \tag{2}$$

Note carefully that all commutators of these row Hamiltonians vanish. (This follows from the fact that for any given atom i the dynamical variables p_i^x and u_i^x appear only in the Hamiltonian for the x row in which its lattice site is situated, and similarly for the variables p_i^y, u_i^y and p_i^z, u_i^z, respectively. Thus, this x-row Hamiltonian commutes with all other x-row Hamiltonians, since they do not contain p_i^x and u_i^x, and also commutes with all y-row and z-row Hamiltonians as they involve p_i^y, u_i^y and p_i^z, u_i^z, respectively.) The Hamiltonian in (2) has the same form as the exactly solvable Mattis–Schultz magnetostriction model for a linear chain.[4] The equivalence of the BE model to a set of $3N^2$ commuting Hamiltonians of the Mattis–Schultz form was noted briefly by BE in a subsequent paper.[6]

Following Mattis and Schultz[4] we remove the mixed terms in (2) involving both the spin and atomic coordinates with the aid of a canonical transformation

$$u_n = q_n + nc + \mu \sum_{m=1}^{n-1} \sigma_m \sigma_{m+1} \ , \tag{3}$$

with p_n left unchanged. For the choice of constants, $c = (F - V')/V''$ and $\mu = J'/V''$, the transformed Hamiltonian is free of terms of the form $(q_{n+1} - q_n)\sigma_n\sigma_{n+1}$ as well as terms linear in $q_{n+1} - q_n$. Specifically, the row Hamiltonian (2) transforms to

$$\mathcal{H} = -\tfrac{1}{2} N \frac{(V' - F)^2 + J'^2}{V''} - (F - V')\left(\frac{J'}{V''}\right) \sum_{n=1}^{N-1} \sigma_n\sigma_{n+1} + \sum_n \left(\frac{p_n^2}{2M} + \frac{1}{2} V''(q_{n+1} - q_n)^2 \right), \tag{4}$$

which describes a harmonic linear chain and an independent spin contribution. The total Hamiltonian (1) of the system is now given by

$$H = H_L + \tilde{H}_I + U, \tag{5}$$

where H_L is the Hamiltonian of $3N^2$ independent harmonic linear chains, $\tilde{H}_I$ is the Ising Hamiltonian for a three-dimensional system of rigid spins interacting via the effective coupling

$$\tilde{J} = J(a) + \frac{(F - V')J'}{V''} \tag{6}$$

and

$$U = -\frac{3}{2} N^3 \frac{(V' - F)^2 + J'^2}{V''} + 3N^3 V(a) \ . \tag{7}$$

Finally, to ensure that the calculated lattice spacing $a + \langle u_{n+1} - u_n \rangle$ equals the actual spacing a, we require[7] that $c + \mu\langle\sigma_n\sigma_{n+1}\rangle = 0$ or, equivalently,

$$F = V'(a) - J'\langle\sigma_i\sigma_j\rangle \tag{8}$$

for a pair of nearest-neighbor spins i, j. The symbol $\langle\;\rangle$ denotes the thermodynamic average taken with respect to the Hamiltonian (5). Equation (8) constitutes the equation of state of the system. With the aid of (8) we can rewrite (6) and (7) as

$$\tilde{J} = \frac{J(a) - J'^2\langle\sigma_i\sigma_j\rangle}{V''} \ , \tag{9}$$

$$U = -\frac{3}{2} N^3 J'^2 \frac{\langle\sigma_i\sigma_j\rangle^2 + 1}{V''} + 3N^3 V(a) \cdot \tag{10}$$

Because of the commutativity of H_L and $\tilde{H}_I$, the quantity $\langle\sigma_i\sigma_j\rangle$ appearing in (8)–(10) is the nearest-neighbor spin-correlation function for the rigid three-dimensional Ising system with the effective exchange coupling $\tilde{J}$. Furthermore, the free energy $\mathfrak{F}$ of the system is given by

$$\mathfrak{F} = U + 3N^2 f_L + \tilde{\mathfrak{F}}_I \ , \tag{11}$$

where f_L is the free energy of a harmonic linear chain of N atoms and $\tilde{\mathfrak{F}}_I$ is the free energy associated with $\tilde{H}_I$. Equations (8)–(11) are the basic equations appearing in the papers of BE and GBI.

In summary, we have presented a new method of solution for the BE model. Our method has not only the important advantage of mathematical simplicity, but it also provides a transparent physical picture of the model system. We utilize the equivalence of the BE model to a set of $3N^2$ linear chains of the Mattis–Schultz type. This equivalence exists as a consequence of the very special form of the BE model. In particular, it is essential that the lattice be chosen as simple cubic and that the interatomic shear terms are excluded from consideration. If either of these features are altered, the correspondence no longer holds and the altered model cannot be diagonalized by any available method.

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[2] M. Fisher, Phys. Rev. 176, 257 (1968).

[3] L. Gunther, D. J. Bergman, and Y. Imry, Phys. Rev. Lett. 27, 558 (1971).

[4] D. C. Mattis and T. D. Schultz, Phys. Rev. 129, 175 (1963); D. C. Mattis, *The Theory of Magnetism* (Harper and Row, New York, 1965), pp. 239–242.

[5] Rather than explicitly include terms in the Hamiltonian to describe the action of external forces, BE evaluate the partition function constraining the surface atoms to their appropriate crystal faces. By contrast, GBI utilize the so-called λ ensemble, which is equivalent to our procedure of utilizing the usual canonical ensemble based on the Hamiltonian of (1). Their parameter λ equals our F.

[6] G. A. Baker, Jr. and J. W. Essam, J. Chem. Phys. 55, 861 (1971).

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Comment on Mills's "Surface Effects in Magnetic Crystals near the Ordering Temperature"

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The Mills result, that the magnetic order at the surface of a semi-infinite crystal appears in a temperature above the Curie point of the infinite crystal, is considered. In the light of this note it is evident that as the Curie point is approached from above the long-range order occurs at one temperature in the whole sample.

Surface effects discussed in one of Mills's recent papers[1] are interesting not only from the point of view of semi-infinite magnetic crystals, but also, and we may even say, first of all, from the point of view of thin-film properties. In the theory of thin films the surface effects and their special role have been known for many years and widely discussed in literature.[2] The equations—based on the effective-molecular-field methods—for magnetization of thin films were introduced by Valenta[3] and developed by Pearson[4] and Wojtczak.[5] From Refs. 2–5 it follows that the spontaneous magnetization of the whole sample disappears in one temperature—contrary to intuitive suggestions given by Brodkorb.[6] A similar situation occurs in the case discussed by Sukiennicki[7] where the spontaneous magnetization of double films coupled by exchange interactions does not vanish locally, but at one temperature corresponding to the Curie temperature of the film with a greater exchange integral.

Since a semi-infinite crystal may be considered as a particular case of a thin film, the results obtained in the thin-film theory refer also to the behavior of spontaneous magnetization at the surface of a semi-infinite crystal. From this point of view we can state that the spontaneous magnetization of a semi-infinite crystal disappears at one temperature. However, Mills reports[1] that from the molecular-field theory it follows that the magnetic order—defined as the average spontaneous magnetization at a lattice site—in a surface layer will appear within the interval of temperatures $T_C < T < T_C^s$ if the exchange integral in a surface layer is sufficiently greater than inside a crystal. T_C^s denotes here a temperature in which the denominator in the formula of the response of the spins in the surface layer to the external field becomes singular and T_C is the Curie temperature of the infinite crystal. A contradiction between the above results inclined us to present this paper.