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1973 J. Phys. A: Math. Nucl. Gen. 6 1527

(http://iopscience.iop.org/0301-0015/6/10/011)

J. Phys. A: Math., Nucl. Gen., Vol. 6, October 1973. Printed in Great Britain.

On the one-dimensional compressible Ising model

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Received 15 January 1973

Abstract. A study of the one-dimensional compressible Ising model, in zero field, with quadratic potential energy and linear exchange parameter, is presented, using a canonical transformation of the hamiltonian. Earlier solutions are corrected and generalized, the role of the four-spin interaction in different ensembles being made explicit. The results agree with the solutions of the Baker–Essam model.

1. Introduction

Several solutions for a compressible Ising model have been suggested during recent years. Domb (1956) showed that, if the exchange parameter J of the Ising hamiltonian is considered as a function of the bulk volume V of the lattice, there is a mechanical instability and the transition becomes of first order. Mattis and Schultz (1963) put forward a theory of elastic induced magnetic transitions and were able to present an 'exact' (ie, taking into account the microscopic position fluctuations) one-dimensional calculation to demonstrate that Domb's model is not good in one dimension at zero pressure. Baker and Essam (1970) worked out a three-dimensional model where the elastic potential energy is quadratic and J linear in terms of the microscopic displacements, and the shear forces are completely neglected; this model is always stable, there is no first order transition, and the one-dimensional version at zero external pressure corresponds to the Mattis solution. Gunther *et al* (1971) used the pressure ensemble to obtain an algebraically simpler solution of the Baker–Essam model. Matsudaira (1968), Wagner (1970), and Bolton and Lee (1970, 1971), with quadratic potential energy, linear J, and zero field, used a canonical transformation to obtain an effective hamiltonian including the long-range interaction of two pairs of spins. Matsudaira, who neglected the influence of transverse phonons, and Bolton and Lee, who used a Debye approximation for the phonon spectrum, worked out mean-field solutions for the transformed hamiltonian at zero pressure. Wagner used the droplet model picture to show that the specific heat at constant vanishing pressure remains finite at the transition temperature.

We think that this sort of transformation of the hamiltonian may be very helpful to investigate the three-dimensional problem more rigorously, and we present here a study of the phase diagram for the one-dimensional case, correcting some results of Bolton and Lee, and showing how to obtain an agreement with the Baker–Essam solution in both canonical and pressure ensembles. For our purposes the classical situation is more convenient to treat, and the quantum treatment of the elastic vibrations should follow analogously.

2. The four-spin transformation of the hamiltonian

The hamiltonian is given by:

$$\mathscr{H} = \Phi + \Psi - K_m X_m + \text{KE}, \tag{2.1}$$

where

$$\Phi = \sum_{(mn)} \phi(X_m - X_n), \qquad \Psi = \sum_{(mn)} -J(X_m - X_n)\sigma_m\sigma_n,$$

$$\phi(X_m - X_n) = \phi_0 + \tfrac{1}{2}\phi_2(X_m - X_n - a_0)^2,$$

and

$$J(X_m - X_n) = J_0 - J_1(X_m - X_n - a_0);$$

ϕ_0, ϕ_2, J_0, J_1 and a_0 are positive constants; K_m are the applied forces and KE is the kinetic energy term. Let us expand this hamiltonian about some equilibrium lattice position R_m such that $X_m = R_m + u_m$. This gives:

$$\mathscr{H} = \text{KE} + \Phi\{R_m\} + \Psi\{R_m\} - K_m R_m + (\Phi^m + \Psi^m - K^m)u_m + \tfrac{1}{2}u_m\Phi^{mn}u_n, \tag{2.2}$$

where Φ^m and Ψ^m are the first derivatives of Φ and Ψ with respect to X_m at the position R_m; Φ^{mn}, the second derivative of Φ, is always a constant. The transformation is straightforward if we write:

$$u_m = v_m + \hat{u}_m \tag{2.3}$$

where

$$\Phi^{mn}\hat{u}_n = -(\Phi^m + \Psi^m - K^m) \tag{2.4}$$

and the usual summation convention is assumed. Using the static Green function for the elastic lattice $G^{mm'}$, where

$$\Phi^{mn}G^{nm'} = -\delta_{m,m'} \tag{2.5}$$

we obtain the transformed hamiltonian, which becomes separated into an elastic and a magnetic part:

$$\mathscr{H} = \text{KE} + \Phi\{R_m\} + \tfrac{1}{2}v_m\Phi^{mn}v_n - K^m R_m + \Psi\{R_m\} + \tfrac{1}{2}(\Phi^m + \Psi^m - K^m)\hat{u}_m \tag{2.6}$$

where

$$\hat{u}_m = G^{mn}(\Phi^n + \Psi^n - K^n). \tag{2.7}$$

At this point there are two distinct choices of boundary conditions: (i) either we can fix the volume (ie the length) of the lattice and work in the usual canonical ensemble (in this case the terms containing the forces should be dropped from the hamiltonian); or (ii) we can let the volume fluctuate and fix the external forces, working in the pressure ensemble. The thermodynamic potential related to the partition function in case (i) is the Helmholtz free energy, and in case (ii) the Gibbs potential; the elastic Green function is going to be quite different for each case, and the four-spin interaction becomes a constant only for fixed forces. The Baker–Essam solution corresponds to situation (i), and the Gunther *et al* solution to situation (ii). In the thermodynamic limit they are related by the usual Legendre transformation.

3. Fixed forces case

In this case either we can have the same force, in opposite directions, applied to both ends of the lattice, or we can fix the initial position and apply a single force to the other end. In the former possibility the centre of mass has to be fixed in order to calculate G^{mn}; however, it is equally simple to obtain the $\hat{u}_m$ through a finite induction procedure and write the four-spin interaction term immediately. We are going to show the solution with the initial position fixed.

Let us first define the expansion positions R_m by the condition

$$\Phi^m - K^m = 0 \qquad \text{everywhere.} \tag{3.1}$$

Then $\{R_m\}$ is not the true equilibrium position of the lattice, but the equilibrium position of the bare elastic lattice, subjected to the same forces. Our hamiltonian becomes:

$$\mathscr{H} = \text{KE} + \Phi\{a\} + \lambda N a + \tfrac{1}{2} v_m \Phi^{mn} v_n + \Psi\{a\} + \text{FSI} \tag{3.2}$$

where λ is the applied force, a is given by equation (3.1), and FSI is the four-spin interaction:

$$\text{FSI} = \tfrac{1}{2} \boldsymbol{\Psi}^{\dagger} \mathbf{G} \boldsymbol{\Psi},$$

in matrix notation. The components of $\boldsymbol{\Psi}$ are $\Psi_i = J_1(\sigma_{i-1}\sigma_i - \sigma_i\sigma_{i+1})$ where $i \in [1, N]$, and $\sigma_{-1} = \sigma_{N+1} = 0$. $\mathbf{G}$ is given by $-\boldsymbol{\Phi}^{-1}$ where it is easy to show that:

$$\boldsymbol{\Phi}^{-1} = \frac{1}{\phi_2} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 2 & 2 & \dots & 2 \\ 1 & 2 & 3 & \dots & 3 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & 2 & 3 & \dots & N \end{pmatrix}.$$

Then it follows:

$$\text{FSI} = -\frac{J_1^2 N}{2\phi_2}, \tag{3.3}$$

and our hamiltonian becomes a simple quadratic elastic part plus an independent Ising magnetic part:

$$\begin{aligned} \mathscr{H} = {} & \text{KE} + \Phi\{a\} + \lambda N a + \tfrac{1}{2}\phi_2\{v_1^2 + (v_2 - v_1)^2 + \dots + (v_N - v_{N-1})^2\} \\ & + \sum_{m=0}^{N-1} -\{J_0 - J_1(a - a_0)\}\sigma_m\sigma_{m+1} - \frac{J_1^2 N}{2\phi_2}. \end{aligned} \tag{3.4}$$

The partition function is:

$$\begin{aligned} Z(\lambda, T) &= \int \prod_i \mathrm{d}p_i \int \prod_i \mathrm{d}v_i \sum_{\{\sigma_m\}} \mathrm{e}^{-\beta\mathscr{H}} \\ &= \left(\frac{2\pi}{\beta\phi_2}\right)^{N/2} Z_1(\beta J_{\text{eff}}) \exp\left\{-\beta N\{\phi_0 + \tfrac{1}{2}\phi_2(a - a_0)^2\} - \beta\lambda N a + \frac{\beta J_1^2 N}{2\phi_2}\right\} \end{aligned} \tag{3.5}$$

where $Z_1(\beta J_{\text{eff}})$ is an Ising partition function calculated at

$$J_{\text{eff}} = J_0 + J_1 \frac{\lambda}{\phi_2}. \tag{3.6}$$

The Gibbs potential is:

$$G(T,\lambda) = N\left(\phi_0 + \lambda a_0 - \frac{1}{2}\frac{\lambda^2 + J_1^2}{\phi_2}\right) - \frac{N}{2\beta}\ln\frac{2\pi}{\beta\phi_2} - \frac{1}{\beta}\ln Z_1(\beta J_{\text{eff}}). \tag{3.7}$$

This result reduces to the Mattis solution if we make $\lambda = 0$. The Baker–Essam model is immediate: the absence of shear forces block-diagonalizes the matrix $\boldsymbol{\Phi}$ for the simple cubic lattice, and each of the identical blocks corresponds to one of the $3N$ lines of atoms of the crystal. If we substitute $3N$ for N in equation (3.7), where N now means the number of unit cells, we regain the Gibbs potential of Gunther *et al*. The real lattice spacing a_R is given by:

$$a_R \equiv \frac{1}{N}\frac{\partial G}{\partial \lambda}\bigg|_T = a_0 - \frac{\lambda}{\phi_2} - \frac{J_1}{\phi_2}\langle\sigma\sigma\rangle_{\text{eff}} \tag{3.8}$$

where the average $\langle\sigma\sigma\rangle_{\text{eff}}$ is a nearest-neighbour spin–spin correlation function calculated with $Z_1(\beta J_{\text{err}})$. In one dimension there is no phase transition, except at zero degrees, when there is a first-order transition at the negative force $\lambda = -J_1\phi_2/J_0$, with a jump in the lattice parameter. It is interesting to point out that: (*a*) Domb's model in one dimension, plus a Maxwell construction, gives a first-order transition at this same pressure, but extending to a temperature range from zero to $T = J_1^2/k\phi_2$; (*b*) a mean-field treatment of the transformed hamiltonian gives the same first-order transition at zero degrees and the usual mean-field second-order transitions at higher temperatures. The Baker–Essam model in three dimensions, in the λ–T plane, has a first-order transition at $\lambda = -J_1\phi_2/J_0$ and $T = 0$, and two lines of second-order Ising transitions for higher temperatures (an antiferromagnetic–paramagnetic transition with J negative, at lower pressures, and a ferromagnetic–paramagnetic transition, with J positive, at higher pressures).

4. Fixed volume case

In order to use the length of the lattice as our parameter, we can either fix the ends or consider periodic boundary conditions for the underlying elastic lattice. Both alternatives lead to the same result, namely that the elastic part of the hamiltonian is again a quadratic form of immediate integration, while the magnetic part, containing two- and four-spin interactions, may be reduced, by means of the σ–τ transformation (see Suzuki 1971), to a well known model solved by Kac (see Stanley 1971). Using periodic boundary conditions, for the purpose of comparing with Bolton and Lee, our hamiltonian becomes:

$$\mathcal{H} = \text{KE} + \Phi\{R_m\} + \tfrac{1}{2}v_m\Phi^{mn}v_n + \Psi\{R_m\} + \text{FSI} \tag{4.1}$$

where the $\{R_m\}$ are now the true equilibrium positions of the lattice, and FSI has the same form as in § 3, with the Green function given by:

$$G^{mn} = -\frac{1}{NM}\sum_{k\neq 0}\frac{e^{ika(m-n)}}{\omega_k^2} \tag{4.2}$$

where M is the ionic mass, a is the lattice spacing, and $\omega_k^2 = (\phi_2/M)(2-2\cos ka)$; the sum is over k in the first Brillouin zone. Bolton and Lee did not exclude the term $k = 0$; hence they did not fix the centre of mass, allowing the presence of a singularity

in the definition of the Green function. This mistake also affects their three-dimensional mean-field calculation. Our four-spin interaction becomes:

$$\text{FSI} = -\frac{1}{2NM}\sum_{k\neq 0}\frac{1}{\omega_k^2}J_1^2\sum_{m,n}\sigma_m\sigma_{m+1}\sigma_n\sigma_{n+1}\,e^{ika(m-n)}(2-2\cos ka). \tag{4.3}$$

Using the property of periodic lattices: $\Sigma_k e^{ika(m-n)} = N\delta_{m,n}$, we have:

$$\text{FSI} = -\frac{J_1^2 N}{2\phi_2}+\frac{J_1^2}{2\phi_2 N}\left(\sum_m \sigma_m\sigma_{m+1}\right)^2. \tag{4.4}$$

The effective magnetic hamiltonian is given by:

$$\mathscr{H}_{\text{mag}} = \sum_m -J(a)\sigma_m\sigma_{m+1} - \frac{J_1^2 N}{2\phi_2}+\frac{J_1^2}{2\phi_2 N}\left(\sum_m \sigma_m\sigma_{m+1}\right)^2. \tag{4.5}$$

The one-to-one σ–τ transformation gives:

$$\mathscr{H}_{\text{mag}} = \sum_m -J(a)\tau_m - \frac{J_1^2 N}{2\phi_2}+\frac{J_1^2}{2\phi_2 N}\left(\sum_m \tau_m\right)^2. \tag{4.6}$$

In this last form of the hamiltonian each spin interacts equally—with an exchange parameter proportional to N^{-1}—with all other spins of the system. Such a model has been studied by Kac, who showed that its exact solution coincides with the conventional mean-field solution. In our case we may suppose that there is a phase transition when the Zeeman term vanishes (ie, when $J(a) = 0$); however, as the exchange parameter is always positive, a simple inspection indicates that there is no such phase transition, except at zero degrees.

In the thermodynamic limit an exact solution for this hamiltonian may be obtained as follows. Let us write $\Sigma_i \tau_i = Nm$; the partition function is:

$$Z = \exp\left(\frac{\beta J_1^2 N}{2\phi_2}\right)\int_{-1}^{+1} dm\, W(m)\exp\left(\beta J(a)Nm - \frac{\beta J_1^2}{2\phi_2}Nm^2\right) \tag{4.7}$$

where

$$W(m) = \frac{N!}{\{\frac{1}{2}N(1+m)\}!\,\{\frac{1}{2}N(1-m)\}!}. \tag{4.8}$$

For N large we can use Stirling's approximation to simplify the expression of $W(m)$ and the integral may be calculated by a saddle-point technique. The stationary point is m_0, $-1 < m_0 < +1$, given by the equation:

$$\beta J(a) - \frac{\beta J_1^2}{\phi_2}m_0 = \tanh^{-1} m_0. \tag{4.9}$$

A graphical analysis of this equation shows that there is only one value of m_0, thus eliminating the possibility of a first-order phase transition. The partition function becomes:

$$Z = \exp\left(\frac{\beta J_1^2 N}{2\phi_2}(1-m_0^2) + N\ln\{2(1-m_0^2)^{-1/2}\} + \frac{Nm_0}{2}\ln\frac{1-m_0}{1+m_0}\right)$$
$$\times \int_{-1}^{+1} dm \exp\left\{-\frac{N}{2}(m-m_0)^2\left(\frac{\beta J_1^2}{\phi_2}+\frac{1}{1-m_0^2}\right)\right\}. \tag{4.10}$$

In the thermodynamic limit we have:

$$\frac{1}{N}F_{\text{mag}} \equiv -\frac{1}{N\beta}\ln Z = -\frac{J_1^2}{2\phi_2}(1-m_0^2)-J(a)m_0$$
$$-\frac{1}{\beta}\ln\{2(1-m_0^2)^{-1/2}\}-\frac{m_0}{2\beta}\ln\frac{1-m_0}{1+m_0}. \tag{4.11}$$

Using equation (4.9) we can write this expression in a more suitable form:

$$\frac{1}{N}F_{\text{mag}} = -\frac{J_1^2}{2\phi_2}(1+m_0^2)-\frac{1}{\beta}\ln\left\{2\cosh\left(\beta J(a)-\frac{\beta J_1^2}{\phi_2}m_0\right)\right\}. \tag{4.12}$$

However, we also have:

$$\langle\sigma\sigma\rangle = \langle m\rangle = \frac{1}{\beta N}\frac{\partial}{\partial J(a)}\ln Z = m_0. \tag{4.13}$$

So the magnetic part of the free energy is finally written as:

$$\frac{1}{N}F_{\text{mag}} = -\frac{J_1^2}{2\phi_2}(1+\langle\sigma\sigma\rangle^2)-\frac{1}{\beta}\ln\left\{2\cosh\left(\beta J(a)-\frac{\beta J_1^2}{\phi_2}\langle\sigma\sigma\rangle\right)\right\} \tag{4.14}$$

where

$$\langle\sigma\sigma\rangle = \tanh\left(\beta J(a)-\frac{\beta J_1^2}{\phi_2}\langle\sigma\sigma\rangle\right). \tag{4.15}$$

For a one-dimensional Ising model, with the hamiltonian $\mathscr{H} = -J_{\text{eff}}\sum_i \sigma_i\sigma_{i+1}$, we have:

$$\frac{1}{N}F_{\text{I}} = -\frac{1}{\beta}\ln(2\cosh\beta J_{\text{eff}}) \tag{4.16}$$

and

$$\langle\sigma\sigma\rangle_{\text{I}} = \tanh(\beta J_{\text{eff}}). \tag{4.17}$$

These relations allow us to write our total expression for the free energy as:

$$F(T,a) = -\frac{N}{2\beta}\ln\left(\frac{2\pi}{\beta\phi_2}\right)+N\{\phi_0+\tfrac{1}{2}\phi_2(a-a_0)^2\}-\frac{NJ_1^2}{2\phi_2}(1+\langle\sigma\sigma\rangle_{\text{eff}}^2)+F_{\text{I}}(J_{\text{eff}}) \tag{4.18}$$

where

$$J_{\text{eff}} = J(a)-\frac{J_1^2}{\phi_2}\langle\sigma\sigma\rangle_{\text{eff}},$$

and $\langle\sigma\sigma\rangle_{\text{eff}}$ is the nearest-neighbour spin–spin correlation function calculated for an Ising model with exchange parameter J_{eff}.

This is the exact result obtainable from Baker and Essam in the one-dimensional case. There is no phase transition, except at zero degrees, when the situation is analogous to the preceding section; the external pressure is given by:

$$\lambda \equiv -\frac{1}{N}\frac{\partial F}{\partial a}\bigg|_T = -\phi_2(a-a_0)-J_1\langle\sigma\sigma\rangle_{\text{eff}} \tag{4.19}$$

and the Gibbs potential is reproduced when we perform the Legendre transformation

$$G(\lambda, T) = F(a, T) + \lambda N a \tag{4.20}$$

with a given by expression (4.19).

5. Conclusions

It is important to observe that, for this simple one-dimensional model, the four-spin interaction has different expressions in the canonical and in the pressure ensembles. In particular it becomes a constant in the pressure ensemble, making it apparent that we do not have to worry about long-range effects; however, this is not so clear in the canonical ensemble. The presence of shear forces in the Baker–Essam model should be investigated, in the pressure ensemble, paying attention to the introduction of additional long-range interactions. It should also be pointed out that some authors, like Wagner, may not be right when they use a pressure ensemble and, at the same time, work with a Green function which is calculated on the basis of periodic boundary conditions.

Acknowledgments

The author acknowledges many helpful discussions with Professor Robert B Griffiths. Comments from Professor J S Langer are also appreciated. During the period this work was done the author was a recipient of a fellowship from FAPESP, Brazil. This work was supported, in part, by a grant from the AFOSR.

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