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Low-Temperature Expansion for Lattice Systems with Many Ground States

J. Slawny[1]

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Low-temperature expansion for systems with many ground states is discussed. It is pointed out that, in general, different ground states may yield different formal perturbation expansions, and that the right expansion of the free energy is provided by ground states called here dominant.

KEY WORDS: Low-temperature expansion; many ground states; dominant ground states.

Low-temperature expansion (LTE) has been used extensively in investigations of magnetic systems and alloys. The LTE is harder to derive and to justify than the high-temperature expansion, which reflects the fact that low-temperature properties are more complicated and interesting than the properties at high temperature. Thus in the past mainly systems of especially simple structure were discussed, systems which are characterized by a high degree of symmetry[(3)] and small number of ground states. The ground states are usually *equivalent* in the sense that they are related by symmetries of the interaction. Ferromagnetic systems are of this kind, and so are antiferromagnetic systems on simple lattices.

To investigate more realistic materials one has to introduce models with more complicated structure.[(9,10,14)] The number of ground states is often large, sometimes even infinite, and the ground states no longer all need to be equivalent (superlattice formation). Below we discuss two examples of such systems, the first one being the nearest neighbor antiferromagnet on a fcc lattice. This model has received considerable attention.[(1–4,9–11,14)] Because of its rich structure and the lack of rigorous results, various authors differ in

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[1] Department of Mathematics, Rutgers University, New Brunswick, New Jersey.

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the interpretation of the numerical material. We obtain rigorous results for stabilizations of this model.

The basis of our work is provided by the recent theory of Pirogov and Sinai.[12] We strengthen slightly some of their results, which allows us to develop systematic perturbation theory around $T = 0$ and to answer the following question: If the ground states are not equivalent, which one should be used in computing the low-temperature expansion? This question is of some importance for numerical calculations since, as we demonstrate below, "natural" choices, such as averaging over ground states[1,4] or using periodic boundary conditions, sometimes lead to wrong coefficients in the expansion.

We discuss in some detail two examples. On the one hand our discussion illustrates the theorem, and on the other hand, it allows us to advance conjectures about some systems with an infinite number of ground states. We give the LTE for the thermodynamic functions only, though Pirogov and Sinai construct a phase diagram at low temperatures: the LTE of the phase diagram is much more involved, and it has not been proved that on some points of the phase diagram the number of phases is not larger than that given by Pirogov and Sinai.

We consider lattice systems with finite-range interactions.

Example 1. The nearest neighbor antiferromagnetic interaction H on a face-centered cubic (fcc) lattice is given by

$$H = J \sum_{\text{n.n.}} \sigma_a \sigma_b$$

where σ_a is the spin-$\frac{1}{2}$ variable at the point a of the lattice, and n.n. indicates sum over pairs a, b of nearest neighbors. Usually, one formulates this model in terms of alloy variables.[9,10,14]

Example 2.[5] The system is located on a simple cubic lattice. The interaction H contains nearest neighbor ferromagnetic interaction and next nearest neighbor antiferromagnetic interaction (Fig. 1):

$$H = -J \sum_{\text{n.n.}} \sigma_a \sigma_b + K \sum_{\text{n.n.n.}} \sigma_a \sigma_b, \qquad J, K > 0$$

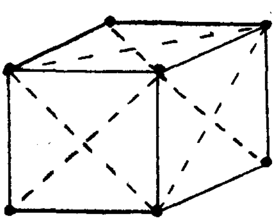

Fig. 1. (——) Ferromagnetic coupling. (---) Antiferromagnetic coupling.

The choice $K = 4J$ yields an infinite number of ground states; see below.

Let now H be any finite-range interaction of a lattice system. By a *ground state* of the system we will understand a configuration which is periodic and for which the energy ϵ_0 per lattice site is minimal. If X is a local perturbation of a ground state Y, i.e., X is equal to Y outside of a finite set, then $H(X|Y)$ will denote its energy with respect to Y. Thus, in Example 1

$$H(X|Y) = \sum_{\text{n.n.}} [\sigma_a(X)\sigma_b(X) - \sigma_a(Y)\sigma_b(Y)]$$

the sum being finite since the expression in brackets is nonzero for a finite number of pairs (a, b) only.

Let $\mathscr{E}$ be the set of all the *excitation energies*:

$$\mathscr{E} = \{H(X|Y): \quad \text{any } Y, X \text{ local perturbation of } Y\}$$

$$\mathscr{E} = \{0, E_1, E_2, \ldots\}, \qquad 0 < E_1 < E_2 < \cdots$$

For a ground state Y let $n_i(Y, \Lambda)$ be the number of perturbations of Y in Λ with energy E_i:

$$\tilde{n}_i(Y, \Lambda) = \text{Card}\{X: \quad H(X|Y) = E_i, \quad X(a) = Y(a), \quad a \notin \Lambda\}.$$

We now make the assumption that for any ground state Y

$$H(X|Y) \to \infty \qquad \text{if} \qquad \text{Card}\{X(a) \neq Y(a)\} \to \infty \tag{1}$$

i.e., when Y is perturbed in large domains the excitation energy becomes large. This assumption is satisfied in systems satisfying the Peierls condition (cf. below), and also in Examples 1 and 2; it is obviously not satisfied by the one-dimensional Ising model in zero external field, or by systems with nonzero ground-state entropy.

Under assumption (1) the $\tilde{n}_i(Y, \Lambda)$ has the following asymptotic behavior as $|\Lambda| \to \infty$: $\tilde{n}_i(Y, \Lambda)$ is a sum of terms which depend on the shape of $|\Lambda|$ and a polynomial in $|\Lambda|$. The coefficient of $|\Lambda|$ in this polynomial, $n_i(Y)$, is called the *multiplicity of E_i in Y*.

If X and Y are ground states, I will say that *X dominates Y in order i* if $n_i(X) > n_i(Y)$, $n_j(X) = n_j(Y)$, $j < i$, and *X dominates Y* if either X dominates Y in a certain order or $n_j(X) = n_j(Y)$ for all j. The X is *dominant* if it dominates any ground state. We let

$$n_j = n_j(X)$$

for any dominant X.

A careful study of ground states and lowest excitations of the model of Example 1 is contained in Ref. 2. The system has six equivalent ground states which possess the translational symmetry of the interaction, and an infinite family of periodic ground states of lesser symmetry. The six ground states dominate the other ground states in order 3:

$$n_1 = 1, \qquad n_2 = 4, \qquad n_3 = 13\tfrac{1}{2} + 2 = 15\tfrac{1}{2}$$

whereas for a ground state Y of period p, i.e., for a ground state invariant under translations by $p\mathbf{i}$, $p\mathbf{j}$, $p\mathbf{k}$ are not invariant under translations by $m\mathbf{i}$, $m\mathbf{j}$, $m\mathbf{k}$ ($|m| < p$),

$$n_3(Y) \leqslant 15\tfrac{1}{2} - 1/p, \qquad p = 2, 3, \ldots$$

The multiplicities can be also obtained by expanding the partition function $Z_\Lambda{}^Y$ of the system in Λ with Y boundary conditions: for low enough temperatures

$$(1/|\Lambda|) \log Z_\Lambda{}^Y = n_0(Y, \Lambda)\beta\epsilon_0 + n_1(Y, \Lambda)e^{-\beta E_1} + n_2(Y, \Lambda)e^{-\beta E_2} + \cdots$$

The multiplicities are the limits of the coefficients of this expansion as Λ becomes large:

$$n_i(Y) = \lim_{\Lambda \to \infty} n_i(Y, \Lambda), \qquad i = 1, 2, \ldots$$

The coefficients $n_i(\text{per}, \Lambda)$ defined in a similar way by imposing the periodic boundary condition will have no limit as Λ increases, unless the multiplicities defined by different ground states are equal.

In the following theorem we assume that the system has a finite number of ground states and that it satisfies the Peierls condition of Refs. 6, 7, and 12 and that therefore the Pirogov–Sinai theory applies. We refer to Ref. 8 for a formulation which is convenient in applications and we note that no system with a finite number of ground states is known for which the Peierls condition does not hold. The free energy of the theorem is the limit, as the volume tends to infinity, of the logarithm of the partition function in a finite volume divided by the number of lattice sites in the volume.

Theorem. (i) The free energy $p(\beta)$, $\beta = 1/KT$, has the following asymptotic expansion as $T \to 0$:

$$p(\beta) \cong \beta\epsilon_0 + n_1 e^{-\beta E_1} + n_2 e^{-\beta E_2} + \cdots + n_k e^{-\beta E_k} + \cdots$$

here ϵ_0 is the ground-state energy per lattice site.

(ii) For low enough temperatures there are (on the Pirogov–Sinai phase diagram) as many pure phases as there are dominant ground states.

Thus, for example, if $n_3(Y) < n_3$ and $n_5(Y) > n_5$ it is not $n_5(Y)$ which appears as the coefficient of $\exp -\beta E_5$, but the smaller multiplicity n_5. Also, the limit of finite-volume states with Y boundary conditions is not expected to yield a pure phase, but to be a mixture of the phases defined by the dominant ground states.

In case of ferromagnetic systems all the ground states are equivalent and stronger results have been obtained. Consider, for example, the two-dimensional Ising model with nearest neighbor interactions J_1, J_2,

$$H = -J_1 \sum_{a\in\mathbb{Z}^2} \sigma_a\sigma_{a+e_1} - J_2 \sum_{a\in\mathbb{Z}^2} \sigma_a\sigma_{a+e_2}$$

In this case the excitation energies E_i are multiples of $2J_1$ and $2J_2$:

$$E_i = k_i 2J_1 + l_i 2J_2$$

where k_i, l_i are positive integers. Thus

$$\exp -\beta E_i = z_1^{k_i} z_2^{l_i}$$

where $z_1 = \exp -2\beta J_1$ and $z_2 = \exp -2\beta J_2$, and the infinite sum in (i) can be written as power series in z_1 and z_2. It appears that the power series converges to $p(\beta) - \beta\epsilon_0$ for sufficiently small z_1 and z_2 and thus $p(\beta) - \beta\epsilon_0$ extends to an analytic function in two complex variables, in some neighborhood of zero. In three dimensions one would obtain analytic function of three variables

$$z_1 = \exp -\beta J_1, \qquad z_2 = \exp -2\beta J_2, \qquad z_3 = \exp -2\beta J_3$$

Similar results hold for any ferromagnetic system, spin $\frac{1}{2}$ and higher spin, the number of variables being equal to the number of nonequivalent bonds.[13] No results of this type are known for general systems of the theorem. It would be of interest to know how to recover $p(\beta)$ knowing the excitation energies E_i and the multiplicities n_i; is the series in (i) summable to $p(\beta)$?

We add a comment on the periodic boundary conditions. They are used to define the coefficients n_i in Ref. 3. As is not hard to see, they provide the right coefficients only in case the ground states have the same multiplicities, as in the case of equivalent ground states; otherwise the periodic boundary conditions will yield wrong coefficients. A similar remark refers to averaging over ground states, as done, for instance, in Refs. 1 and 4.

Extending the theorem, we can also give a perturbation expansion for the phase diagram of the Pirogov–Sinai theory. Since its formulation is much more involved, we will present it on another occasion.

I shall now illustrate the theorem by applying it to the Examples. I am especially interested here in using it to arrive at conjectures at what happens for those values of the parameters for which the number of ground states is infinite. Since the theorem requires the number of ground states to be finite, I introduce first perturbations reducing the number of ground states. Let m

be a positive integer and let us change the interaction by adding the ferromagnetic interaction

$$-M \sum_{a \in \mathbb{L}} \sigma_a(\sigma_{a+me_1} + \sigma_{a+me_2} + \sigma_{a+me_3}), \qquad M \geqslant 0$$

This perturbation (stabilization) eliminates the ground states not invariant under translation generated by me_1, me_2, me_3.

Example 1 (cd). The stabilized interaction is

$$J \sum_{\text{n.n.}} \sigma_a\sigma_b - M \sum_a (\sigma_a\sigma_{a+me_1} + \sigma_a\sigma_{a+me_2} + \sigma_a\sigma_{a+m_3})$$

It has approximately $3\cdot(2m)!$ ground states. For any ground state X the excitation energies split under the perturbation as follows: E_i splits into $E_{ij}(M)$, $j = 1,..., k_i$,

$$E_{ij}(M) = E_i + \eta_{ij}M, \qquad \eta_{ij} \geqslant 0$$

with

$$n_i(X) = \sum_{j=1}^{k_i} n_{ij}(X)$$

where $\eta_{ij}(X)$ are M-independent for small enough M. Easy calculation yields $k_1 = 1$, $k_2 = 1$ (no splitting of the first two energy levels),

$$E_{11}(M) = E_1 + 2M, \qquad E_{21}(M) = E_2 + 4M$$

for *each periodic ground state* X. It follows that for small enough M the six ground states, and only those, are dominant, and, by the Theorem, determine the asymptotic expansion of p:

$$p(\beta, M) \cong \beta\epsilon_0(M) + \left(\sum_{j=1}^{k_1} n_{1j}e^{-\beta E_{1j}(M)}\right) + \left(\sum_{j=1}^{k_1} n_{2j}e^{-\beta E_{2j}(M)}\right) + \cdots$$

As $M \to 0$ the RMS here goes over into

$$\beta\epsilon_0 + n_1e^{-\beta E_1} + n_2e^{-\beta E_2} + \cdots$$

where n_i are the multiplicities of the six ground states. This differs from the expansion of Refs. 1 and 4, where n_i are equal to an average of the multiplicities $n_i(X)$ over X.

The same argument yields only six pure phases for any $M > 0$ in spite of the large number of ground states. We conjecture that this is the situation for $M = 0$, too. Using the reflection positivity property of the model, I have shown that at $M = 0$ there are at least six equilibrium states. However, this does not prove that there is more than one *invariant* equilibrium state, i.e., that there is a first-order phase transition at low temperatures.

Example 2 (cd). For $K < 4J$ there are two equivalent ground states E, F: $E_a = +1$ all a, and $F_a = -1$ all a. Correspondingly, at low temperature there are two pure phases. For $K > 4J$ there are six ground states, all equivalent, and six pure phases at low temperatures; each of the six ground states has period 2. For $K = 4J$, apart from the eight ground states above, there is an infinite family of ground states of lesser symmetry each obtained from E (or F) by flipping spins in planes perpendicular to one of the coordinate axes.[5] States E and F are equivalent and, as can be shown, dominate any other ground state in order 1. Thus I expect to have only two phases at low temperature and the asymptotic expansion given by E (and F). Again as in the first example exactly such a picture obtains if long-range stabilization is introduced.

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