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Phase Transitions in New Solvable Hamiltonians by a Hamiltonian Minimization

Mehran Kardar
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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By minimization of a Hamiltonian with respect to its interaction parameters, new Hamiltonians are generated. The same minimization procedure is carried out with the free energy of the initial Hamiltonian, and it is proven that in the thermodynamic limit the minimized free energy is the free energy of the minimized Hamiltonian. This method is illustrated with two-dimensional Ising models generalized to include both nearest-neighbor bonds and infinite-range bond-bond interactions. New critical behavior is observed.

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There are only a limited number of phase-transition problems, such as the two-dimensional Ising and vertex models, for which exact solutions to the free energy are known.[1] In this paper, a method is proposed for obtaining new solvable Hamiltonians by generalizing Hamiltonians that are solvable. As an application of this method, the nearest-neighbor Ising model is generalized to also include infinite-range bond-bond interactions. Similar Hamiltonians have been encountered in the context of compressible Ising models.[2-4] New critical behavior is observed in the vicinity of the Ising critical point. A general feature of this procedure is that the new interactions generated are of infinite range, and thus it is particularly suitable to the study of competing short-range and long-range interactions.

The interaction parameters of a Hamiltonian can be made functions of a set of variables. A formal minimization of the Hamiltonian with respect to these variables generates new Hamiltonians in which the operators are functions of the operators in the initial Hamiltonian. It is proven that in the thermodynamic limit the operations of taking the thermodynamic trace and maximizing the partition function commute. Thus, the free energy of the new (minimized) Hamiltonians is simply obtained by minimizing the free energy of the initial Hamiltonian with respect to the same set of variables. Manipulating the free energy close to a critical point can change the nature of the phase transition.[5,6] For example, hidden variables that put constraints on a Hamiltonian can cause renormalization of exponents.[5] Minimizing the free energy can result in similar changes. However, the minimized free energy now corresponds to a real Hamiltonian.

Consider a Hamiltonian $\mathcal{H}_0(x)$, describing a system of N *discrete classical* spins, in which the energy levels $E_n(x)$ are functions of a variable x. Such a variation in energy levels can be obtained by making the interaction parameters dependent on x. The partition function obtained by summing over all possible spin configurations will also depend on x,

$$Z_0(x) = \mathrm{Tr}\{\exp[-\mathcal{H}_0(x)]\} = \sum_n g_n \exp[-E_n(x)], \quad (1)$$

where $\{g_n\}$ are the degeneracies of the energy levels (a factor of $\beta = 1/kT$ is absorbed into $\mathcal{H}_0$). For the simple discrete-spin systems considered in this paper, such as Ising and Potts models in a uniform field, the degeneracies g_n are independent of x (apart from the trivial cases of energy crossing). Also, we consider only cases where each energy level $E_n(x)$ is minimized for a single value x_n, such that $\partial E_n/\partial x = 0$ at $x = x_n$. The set of minimized energy levels $\{E_n(x_n)\}$ describe a new Hamiltonian $\hat{\mathcal{H}}$, which will be referred to as the minimized Hamiltonian. The $\{x_n\}$ can be regarded as the values of an operator $\hat{x}$ that minimizes $\hat{\mathcal{H}}_0(x)$, i.e., the solution to $\partial\hat{\mathcal{H}}_0/\partial x|_{x=\hat{x}} = 0$. The minimized Hamiltonian is obtained by substituting the operator $\hat{x}$ in the original Hamiltonian, $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0(\hat{x})$. This operation simply puts together the minimization of the individual levels, and will be clarified by actual examples further on. The partition function of the minimized Hamiltonian is

$$Z = \mathrm{Tr}\{e^{-\hat{\mathcal{H}}}\}$$
$$= \sum_n g_n \exp[-E_n(x_n)] \underset{N\to\infty}{\simeq} g_a \exp[-E_a(x_a)], \qquad (2)$$

where the subscript a denotes the dominant term in the sum. Indeed, in the thermodynamic limit ($N\to\infty$) this largest term is sufficient to describe the partition function.[7] This result is valid as long as $\lim_{N\to 0}(\ln\mathfrak{N})/N = 0$, where $\mathfrak{N}$ is the number of energy levels. The original partition function $Z_0(x)$, on the other hand, is maximized for a particular value $\bar{x}$:

$$Z_0(\bar{x}) = \sum_n g_n \exp[-E_n(\bar{x})] \geq Z_0(x). \qquad (3)$$

Since each x_n minimizes $E_n(x)$, each term in the sum in Eq. (2) is larger than or equal to the corresponding term in Eq. (3), and hence $Z \geq Z_0(\bar{x})$. But $\bar{x}$ maximizes $Z_0(x)$ and hence

$$Z \geq Z_0(\bar{x}) \geq Z_0(x_a) \geq g_a \exp[-E_a(x_a)]. \qquad (4)$$

In the thermodynamic limit, $Z = g_a \exp[-E_a(x_a)]$. Hence, it is proven that in this limit $Z = Z_0(\bar{x})$; that is, the partition function (or free energy) of the minimized Hamiltonian $\hat{\mathcal{H}}$ is given by the maximized partition function (or minimized free energy) of the original Hamiltonian $\hat{\mathcal{H}}_0(x)$. In other words, in the thermodynamic limit the operations of taking the trace and maximizing with respect to x commute with each other:

$$Z = \mathrm{Tr}(\max\{\exp[-\hat{\mathcal{H}}_0(x)]\}_x)$$
$$= \max(\mathrm{Tr}\{\exp[-\hat{\mathcal{H}}_0(x)]\})_x. \qquad (5)$$

This result reflects the fact that taking the thermodynamic trace is just another maximization of $g_n \exp[-E_n(x)]$ with respect to n, which obviously commutes with the other maximization with respect to x. The value of $\bar{x}$ that maximizes $Z_0(x)$ is the expectation value of the operator $\hat{x}$ in the Hamiltonian $\hat{\mathcal{H}}$. With some modifications these results can be generalized to a set of variables $\{x_i\}$, and to continuous-spin systems. A number of examples will now be considered in order to illustrate this method and its applications.

The simplest example of this method is the derivation of the familiar equations of mean-field theory starting with a Hamiltonian $\hat{\mathcal{H}}_0(x) = Nx^2/2J - (h+x)\sum_i \sigma_i$, describing a set of N decoupled Ising spins. The Hamiltonian has $N+1$ energy levels depending on the magnetization $m = \sum_i \sigma_i$. The energy levels $E_m(x) = Nx^2/2J - (h+x)m$ each have a minimum at $x_m = (J/N)m$, and the corresponding degeneracies

$$g_m = \binom{N}{(N-m)/2}$$

are manifestly independent of x. The minimized energy levels are $E_m(x_m) = -(J/2N)m^2 - hm$. The minimized Hamiltonian is obtained by setting $\partial\hat{\mathcal{H}}_0/\partial x|_{x=\hat{x}}$ equal to zero as

$$\hat{x} = \frac{J}{N}\sum_i \sigma_i;$$
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0(\hat{x}) = -\frac{J}{2N}\sum_{i,j}\sigma_i\sigma_j - h\sum_i \sigma_i. \qquad (6)$$

The Hamiltonian $\hat{\mathcal{H}}$ describes an Ising model subject to equivalent-neighbor interactions $(J/N)\sigma_i\sigma_j$. The free energy for $\hat{\mathcal{H}}_0(x)$ is

$$F_0(x) = N[x^2/2J - \ln 2\cosh(h+x)],$$

and hence the free energy for $\hat{\mathcal{H}}$ is given by

$$F = N \min[x^2/2J - \ln 2\cosh(h+x)]_x, \qquad (7)$$

which is clearly the mean-field-theory expression for the free energy of the Ising model. The relation between the equivalent-neighbor Ising model and mean-field theory is well known.[8]

In the above example the initial Hamiltonian involved an operator $\hat{\mathcal{O}} = \sum_i \sigma_i$, while the minimized Hamiltonian included the additional operator $\hat{\mathcal{O}}^2 = \sum_{i,j}\sigma_i\sigma_j$. This new (equivalent-neighbor) interaction can be used in the study of competition between short-range and long-range forces. Such competition has been studied in other contexts by different (and often more cumbersome) methods.[9,10] Similarly, various other powers and functions of $\hat{\mathcal{O}}$ can be constructed. The operator $\hat{\mathcal{O}}^3$, for example, corresponds to three-point interactions, while $|\hat{\mathcal{O}}|^{3/2}$ cannot be regarded as a simple interaction, although it is a legitimate many-body operator. If the initial Hamiltonian includes operators $\hat{\mathcal{O}}_1$ and $\hat{\mathcal{O}}_2$, the minimized Hamiltonian can include products of these operators.

The main difference between this method and traditional forms of mean-field theory[11] is that the function to be minimized does not have to be analytic [and indeed will have nonanalytic terms if $\hat{\mathcal{H}}_0(x)$ has phase transitions], and hence new forms of critical behavior not encountered in mean-field theory can be observed.[12] Also, this result provides a clear and direct method for obtaining the Hamiltonian, and the free energy that describes it exactly.

A nontrivial example is provided by the nearest-neighbor Ising models generalized in the same fashion. Starting with a Hamiltonian

$$\hat{\mathcal{H}}_0(x) = \frac{Nx^2}{2J} - (K+x)\sum_{\langle ij\rangle}\sigma_i\sigma_j,$$

the minimized Hamiltonian is given by

$$\hat{\mathcal{H}} = -K\sum_{\langle ij\rangle}\sigma_i\sigma_j - \frac{J}{2N}\sum_{\langle ij\rangle,\langle kl\rangle}\sigma_i\sigma_j\sigma_k\sigma_l, \qquad (8)$$

describing the nearest-neighbor Ising model subject to additional infinite-range bond-bond interactions. Such interactions do arise and have been studied in the context of compressible Ising models.[13,14] The free energy per spin is

$$f(J,K) = \min[f_0(K+x) + x^2/2J]_x, \qquad (9)$$

where f_0 is the free energy of the nearest-neighbor Ising model. The optimal value of x is the solution of

$$\bar{x} = -Jf_0'(K+\bar{x}). \qquad (10)$$

In particular, we consider the cases of the one-dimensional Ising model,[15] and the two-dimensional Ising models on the square[16] and triangular lattices[17] for which exact solutions are known. Phase diagrams are given in Fig. 1. {The one-dimensional problem can be mapped onto the Hamiltonian in Eq. (6) by a simple change of variables and is not particularly interesting [Fig. 1(a)].} The phase diagram on the square lattice [Fig. 1(b)] exhibits a triple point separating the ferromagnetic, antiferromagnetic, and paramagnetic phases. The transitions from the disordered phase to the ordered phases are first order except for $J=0$. The corresponding phase diagram

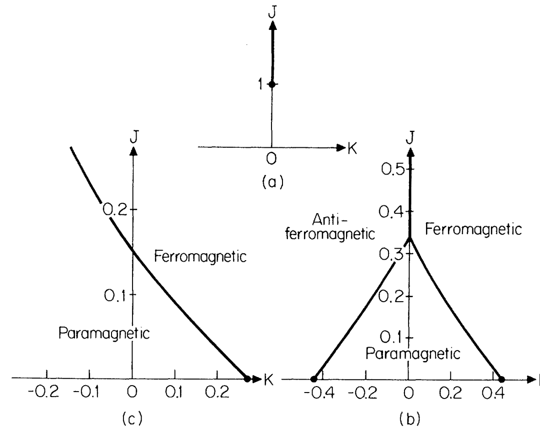

FIG. 1. Phase diagrams for Ising models with nearest-neighbor interaction K, and infinite-range bond-bond coupling J/N. Solid lines are first-order transitions terminating at critical points. (a) One-dimensional lattice, (b) square lattice, and (c) triangular lattice.

for the triangular lattice [Fig. 1(c)] has a different structure. This results from frustration in the triangular antiferromagnetic Ising model, which stays disordered down to zero temperature. However, the antiferromagnet undergoes a first-order transition to a ferromagnetic state for sufficiently large values of the bond-bond interaction term. The gradient of the first-order phase boundary (PB) is given by

$$\partial K/\partial J|_{\mathrm{PB}} = \tfrac{1}{2}[f_0'(\bar{x}_1+K) + f_0'(\bar{x}_2+K)], \qquad (11)$$

where $\bar{x}_1$ and $\bar{x}_2$ are the positions of the two minima that cross causing the phase transition. The derivatives of the free energy are given by

$$\partial f/\partial k = f_0'(\bar{x}+K),$$
$$\partial^2 f/\partial K^2 = \frac{f_0''(\bar{x}+K)}{1+Jf_0''(\bar{x}+K)}. \qquad (12)$$

The vicinity of the critical point of the pure Ising model at $J=0$ and $K=K_c$ is particularly interesting. An expansion of the free energy around this point becomes nonanalytic, resulting in new critical behavior. In fact, an expansion of $f_0(K+x) + x^2/2J$ in the small parameter $t = K + x - K_c$ gives

$$f(J,K) = \min\{-b + [f_0'(K_c) + (K_c - K)/J]t - ct^2|t|^{-\alpha} + t^2/2J\}_t, \qquad (13)$$

where b and c are constants and α describes the singularity in $f_0''(t)$. The expression to be minimized is different from those encountered in mean-field theory in that it is explicitly nonanalytic in t. As the critical point is approached along the first-order phase boundary the response function $\partial^2 f/\partial K^2$ diverges as $(1-\alpha)/\alpha J$, and the critical behavior makes a crossover from Ising to first-order behavior for $\delta K \sim J^{1/\alpha}$. In the case of the two-dimensional Ising models where $\alpha = 0$ (logarithmic divergence),

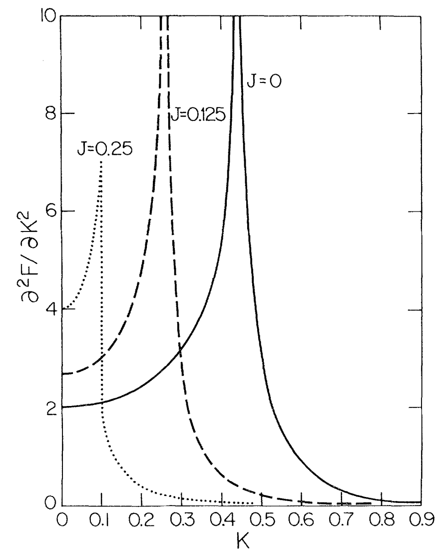

FIG. 2. The response function $\partial^2 f/\partial K^2$ as a function of K for $J=0$, 0.125, and 0.25.

$\partial^2 f/\partial K^2$ diverges as $1/J^2$, and the crossover region is exponentially small, $\delta K \sim \exp(-c/J)$. Figure 2 shows $\partial^2 f/\partial K^2$ for the square lattice as a function of K for various VOLUME of J. Note that maximizing Eqs. (9) or (13) for negative J leads to a continuous transition with renormalized exponents. However, it is not clear that the maximized free energy indeed describes any physical Hamiltonian.[17]

In summary, I have presented a new result in statistical mechanics that can be used to generalize certain Hamiltonians, and to obtain the corresponding free energies. Application of this method to Ising models results in new critical exponents describing the crossover between transitions dominated by short-range and infinite-range interactions. This procedure can describe the crossover from Ising to mean-field criticality on Bravais lattices,[18] and on the Cayley tree where the competition between the two types of interaction results in rich new critical behavior resembling a system of variable dimensionality.[12] This type of competition can also be studied in Potts models and percolation problems.[19] There are also applications of this method in frustrated Ising systems, and also in applying nonlocal constraints to Hamiltonians.[19]

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$$\frac{\ln x_a}{N} \leqslant \frac{\ln Z}{N} \leqslant \frac{\ln x_a}{N} + \frac{\ln \mathfrak{N}}{N}.$$

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