Bethe or Bethe-like Lattice Calculations Are More Reliable Than Conventional Mean-Field Calculations

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We demonstrate that the behavior on Bethe or Bethe-like lattices are qualitatively correct even when conventional mean-field theories fail. We also give a new and direct method for calculating the bulk free energy ω_B for any model on a recursive lattice.

There are two types of mean-field approximations in use. In the conventional type, as formalized by Landau [1], one introduces an order parameter, but correlations between fluctuations at different sites are *neglected*. However, the lattice geometry is not distorted. In the other type, the lattice is approximated by a (Cayley) tree [2], but the resulting problem is solved *exactly*, including correlations except that they are weak. (A Cayley tree $\Im$, Fig. 1, possesses a *surface* with a nonzero density of sites, even if $\Im$ is infinitely large. The Bethe lattice is the infinite "interior" of the infinite tree and has *no* surface.) While the behavior in the interior of $\Im$ is similar to that predicted by conventional mean-field theories in many cases, we shall demonstrate here that this is not true in general. On the other hand, the behavior on the entire tree can be strange and very different from those on regular lattices [3]. This is due to a finite surface site density on $\Im$.

Conventional mean-field theories are not always trustworthy. According to Netz and Berker [4], the failure in the case of a triangular antiferromagnet Ising model is due to a violation of the hard-spin condition $S^2 = 1$ which is critical for incorporating *frustration* [5]. They also fail in gauge theories [6] by violating Wegner-Elitzur theorem [7], presumable because gauge symmetries are no longer intact due to lack of correlations. Since the calculations on a tree or any other recursive structure are done exactly, whether frustrations or gauge symmetries are present or not, we may ask: "Are the predictions on a Bethe lattice or a similar recursive structure more reliable in general?"

We consider frustrations, gauge symmetries, etc., as part of a general scenario. We shall demonstrate that the answer is *affirmative*. Therefore, in order to make such calculations *complete*, we shall also provide a direct and elegant method of computing the (bulk) free energy ω_B in the interior. This free energy must be *insensitive* to a wide variety of surface conditions, which is what happens on regular lattices. The knowledge of ω_B is critical for locating phase transitions in case of multiple solutions to the equation of state (EOS) and for determining the equilibrium state.

The calculation on a tree is done *recursively*. It is a standard and well-known [3] method. Therefore, we will merely sketch it below and refer the reader to Ref. [8] for more details. The tree is divided into generations [8], $m = 0$ being the origin and $m = M$ being the *surface;* the tree with the center at $m = 0$ and the surface at $m = M$ is denoted by $\Im_{0,M}$. Let q denote the coordination number. On each site is a spin S (not necessarily Ising) and τ denotes the set of nearest-neighbor (nn) $r = q - 1$ spins on $(m + 1)$st generation. Let $Z_m(S)$ denote the restricted partition function (PF) obtained by summing over *all* spins on higher generations that lie between S and the surface. The recurrence relation (RR) between Z_m and Z_{m+1} is

$$Z_m(S) = \mathrm{Tr}\, W(S, \tau) \prod_{T \in \tau} Z_{m+1}(T), \qquad (1)$$

where $W(S, \tau)$ denotes the Boltzmann weight due to interactions between S and τ and between τ and external fields. Tr denotes the trace over spin states of all $T \in \tau$. Using (1) recursively, we obtain $Z_0(S)$, the restricted PF for one of the q bonds meeting at the origin (Fig. 1). Hence, the total PF is
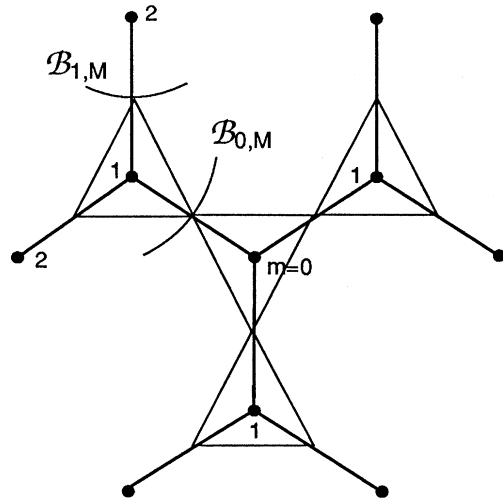
$$Z_{0,M} = \mathrm{Tr}\, W(S) \prod Z_0(S), \qquad (2)$$

FIG. 1. A portion of a Cayley tree of coordination $q = 3$, with branches $\mathcal{B}_{0,M}$ and subbranches $\mathcal{B}_{1,M}$. The cactus shown by light lines is obtained by connecting nn bonds.

for the tree $\mathfrak{S}_{0,M}$. Here, $W(S)$ denotes the Boltzmann weight for the interaction between S and external fields, Tr denotes the trace over spin states of S, and the product is over the q bonds at the origin. Obviously, $Z_{0,M}$ depends on the *initial* or *surface* condition $Z_M(S)$. This procedure gives the free energy ω per bond for the entire tree $\mathfrak{S}_{0,M}$, even as $M \to \infty$, and is *exact*.

It is known [3] that ω gives rise to unusual behavior due to surface sites. In particular, it depends on *surface* conditions. On the other hand, we demand that the bulk free energy ω_B per bond must be *independent* of a wide class of surface conditions. The difference $\omega - \omega_B$ yields the surface contribution ω_S to the free energy and contains the entire effect of the surface. For realistic lattices, ω_S vanishes in the thermodynamic limit and $\omega = \omega_B$. This does not happen for trees and, therefore, ω and ω_B are usually *different*, with ω surface dependent and ω_B surface independent.

To obtain ω_B, we must get rid of the surface contribution which is not trivial. The procedure for ferromagnetic Ising model is described by Baxter [9]: One integrates the EOS with respect to the field to obtain the free energy. One also makes use of the following homogeneity assumption: $b = q/2$ for the ratio of bonds to site in the interior, even though $b = 1$ for an infinite tree. An alternative approach is to calculate the entropy and the energy in terms of an order parameter [10], use $b = q/2$, and minimize the free energy with respect to the order parameter. However, the homogeneity assumption has been questioned by Eggarter [3]. Also, as shown by Bowman and Levin [11], using $b = q/2$ yields unphysical results for the spin-glass problem. There are other drawbacks of the above two approaches: (i) EOS may not be known for all fields; (ii) EOS may not be easily integrable; (iii) the order parameter may not be known, etc.

We describe a new and direct approach to calculate ω_B which neither requires the knowledge of the order parameter nor the integration. Further, no homogeneity assumption is made. It, nevertheless, comes out as a consequence of our procedure. The method is general and applicable to any system with any surface condition and is valid for all recursive lattices. The generality of our method makes it very useful and important. Our method reproduces the free energy in cases where it is known by other methods. This includes the Ising model discussed by Baxter. In cases where the free energy is not known by other methods, our method allows for its evaluation. These include polymers among others.

Consider a tree $\mathfrak{S}_{0,M}$ with the origin at $m = 0$ and the surface at $m = M$. The tree is obtained by "hooking" q different branches $\mathfrak{B}_{0,M}$ at the origin (Fig. 1). Each $\mathfrak{B}_{0,M}$ can be divided into $r = q - 1$ subbranches $\mathfrak{B}_{1,M}$ that are connected by a bond to a site on $m = 1$ generation. The difference δ between the number of bonds on q $\mathfrak{B}_{0,M}$ branches and rq $\mathfrak{B}_{1,M}$ branches is the q bonds meeting at the origin: $\delta = q$. Now, consider the union $\mathfrak{S}'_{1,M}$ of r different trees $\mathfrak{S}_{1,M}$, each formed by hooking q different

subbranches $\mathfrak{B}_{1,M}$. Let $Z_{0,M}$ and $Z^{(i)}_{1,M}$, $i = 1, 2, \ldots, r$, denote the PF's of $\mathfrak{S}_{0,M}$ and each of $\mathfrak{S}_{1,M}$, respectively. Then, as $M \to \infty$,

$$\omega_B = \lim_{M \to \infty} (1/\delta) \left[\ln Z_{0,M} - \sum_{i=1}^{r} \ln Z^{(i)}_{1,M} \right] \qquad (3)$$

gives the *bulk* free energy per bond at the origin, and can be calculated for any model (Ising, Potts, gauge, polymers, etc.) whether pure or random, *provided* there is a fixed point (FP) or a fixed-point distribution function of the EOS at the origin. The procedure can be carried out on any recursive lattice. Since the FP is insensitive to a wide class of surface conditions, the resulting bulk free energy in (3) is also independent of this class.

From Fig. 1, we also note that the $\mathfrak{S}_{0,M}$ and the union $\mathfrak{S}'_{1,M}$ also differ by two sites only as can be easily checked. Hence, $q\omega_B$ is also equal to twice the bulk free energy per site. In other words, $b = \delta/2 = q/2$, as expected. It should also be evident that one can also compare $\mathfrak{S}_{0,\infty}$ with a proper union $\mathfrak{S}'_{k,\infty}$ of qr^{k-1} different trees $\mathfrak{S}_{k,\infty}$ with $k \to \infty$. Here, $\mathfrak{S}_{k,\infty}$ denotes a tree with the origin at $m = k$ and the surface $M = \infty$. Then, a subtraction similar to (3) divided by qr^{k-1} gives ω_B per bond for a *macroscopic* and *homogeneous* interior of $\mathfrak{S}_{0,\infty}$, which is the Bethe lattice. What we have shown is that one can take $k = 1$ also, which makes computation much simpler, especially when randomness is present. However, we are interested only in pure systems here.

By a *proper* choice of $Z_M(S)$ at the surface, one can make ω per bond obtained from (2) to be identical to ω_B, see example (A) below. However, this makes the surface contribution to be *temperature dependent*. In that case, care must be exercised in calculating quantities like entropy which requires temperature derivatives [11]. Consider, for example, an Ising model and write $Z_M(S) = \exp(-\beta\varepsilon_S + H_S S)$ at each surface site. The PF is

$$Z_{0,M} = e^{-\beta E_S} \sum \Omega(E, M_S) e^{-\beta E + H_S M_S},$$

where $E_S = N_S \varepsilon_S$ (N_S being the number of surface sites) and H_S are surface energy and field determined by $Z_M(S)$, E and M_S are the energy and surface magnetization in a given configuration, and Ω is the number of configurations for a given E and M_S. Usual thermodynamic arguments show that the "free energy" $S - \beta E + H_S M_S$, $S = \ln \Omega(E, M_S)$, must be maximized as a function of E and M_S to yield ω_B. Therefore, the equilibrium state must be stable. Furthermore, since $\Omega \geq 1$, $S \geq 0$. Thus, ω_B must satisfy all the requirements of equilibrium thermodynamics. The simplest way to obtain S is to perform the Legendre transform:

$$S = \omega_B + \beta\overline{E} - H_S\overline{M}, \qquad (4)$$

where $\overline{E}, \overline{M}_S$ are the equilibrium values.

We now turn to various examples.

(A) Ising model with nn interactions.—The reduced Hamiltonian $\mathcal{H} = -\beta E = K \sum S_i S_j + H \sum S_i$. Let $u = e^K$ and $v = e^H$. We consider the model on the tree

in Fig. 1 with arbitrary q. We set $Z_m(1) = B_m x_m$ and $Z_m(-1) = B_m$. From (1), we find that the RR's are

$$B_m = B_{m+1}^r f(x_{m+1}), \quad x_m = g(x_{m+1})/f(x_{m+1}), \quad (5)$$

where $g(x) = uvx^r + 1/uv$, $f(x) = g(x)$ with $u \rightarrow 1/u$. The RR for x_m is also called the EOS. The PF at the origin is $Z_{0,M} = B_0^q y(x_0)$ with $y(x) = vx^q + 1/v$, and the magnetization μ_0 at the origin is $(vx_0^q - 1/v)/y(x_0)$. The free energy is

$$\omega_B = (1/q) \ln\left(B_0^q y(x_0)/[B_1^q y(x_1)]^r \right). \quad (6)$$

As $M \rightarrow \infty$ and $K > 0$, we obtain $x_0 = x_1 = x$, a FP for the RR of x_m, and ω_B reduced to $\omega_B = \ln f(x)/[y(x)]^{(q-2)/q}$. A little bit of algebra shows that this is $b = q/2$ times the free energy per site given by Baxter [9]. (Note that our x is the inverse of x used by Baxter.)

By expressing B_0 recursively in terms of B_M, it is easy to show that when $x_M =$ FPx of the EOS, $\omega = \omega_B$ provided $B_m^q = 1/y(x)$. Thus, it is *not* sufficient to set $x_M =$ FPx, to ensure $\omega = \omega_B$; one must also choose B_M appropriately. This makes $Z_M(S)$ temperature dependent. The above choice of B_M ensures that $\mathfrak{S}_{0,M}$ itself can be thought of as a part of a larger tree $\mathfrak{S}_{0,M'}$, $M' > M$, and that the free energy of the portion of the tree outside of $\mathfrak{S}_{0,M}$ is *zero*. This is because this outside portion can be thought of as giving rise to a large number of trees $\mathfrak{S}_{M,M'}$ and the PF for a tree $\mathfrak{S}_{M,M'}$ is $Z_{M,M'} = B_M^q y = 1$, see (2). Hence, the free energy for this tree is zero.

(B) Frustration.—For $K < 0$, one can solve the Ising model above by making the substitution $S \rightarrow -S$ on alternate generations. Since there is *no* frustration on the tree (Fig. 1), the problem is of no interest. To ensure the presence of frustration, we consider the "cactus" shown in Fig. 2, where each site has six neighbors (as on a triangular lattice) and the three spins on each triangular plaquette interact pairwise. We consider $H = 0$. The frustration is inherent and cannot be removed. Let $Z_m(S) = B_m x_m^{(S+1)/2}$ be the restricted PF of a spin S on
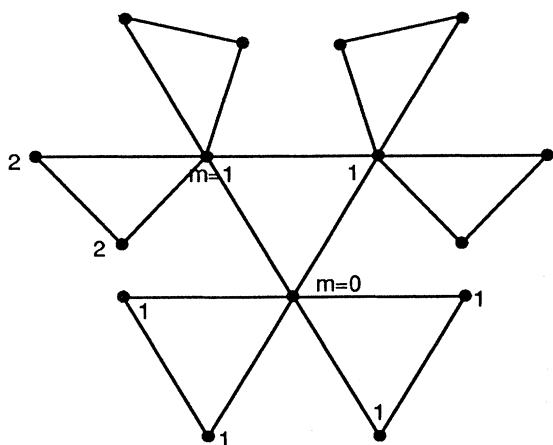
a triangle. We find that $(u = e^{-K})$:

$$B_m = B_{m+1}^4 f(x_{m+1}), \quad x_m = g(x_{m+1})/f(x_{m+1}),$$

with $f(x) = (x^4 + 2x^2)u + 1/u^3$, $g(x) = x^4 f(1/x)$. The RR for x_m always has $x_m = 1 = x_{m+1}$ as a FP solution and corresponds to a zero magnetization: $\mu_0 = (x_0^3 - 1)/(x_0^3 + 1) = 0$.

We now study the stable state at absolute zero $(T = 0)$ to see if there is a phase transition. For a given spin state $S = 1$ (or -1) at m, the two spins on the same triangle at $m + 1$ are either (i) both $S = -1$ (or $+1$) or (ii) opposite to each other. Both have identical energies but the state (ii) has more entropy; therefore, we expect this to yield the stable state. The magnetization in the state (i) alternates between generations $(x_m = 1/x_{m+1})$, while in the state (ii) is zero everywhere: $x_m = x_{m+1} = 1$. Thus, we do not expect any phase transition, even at $T = 0$.

To confirm this, we set $x_1 = 1/x_0$ in the RR for x_0. For $u \rightarrow \infty$, $x_0 \sim u^4$, and is *different* from $x_0 = 1$. This suggests a possible phase transition. To investigate this, we must compare the free energies. This example also shows why knowing ω_B is essential. The free energy per plaquette is $\omega_B = (\frac{1}{3}) \ln z$, $z = B_0^3 y(x_0)/[B_1^3 y(x_1)]^4$ since there are 12 plaquettes coming in at $m = 1$ and we need only three plaquettes to meet at $m = 0$. Here, $y(x) = x^3 + 1$. For $x_0 = 1/x_1 = 1$, $z \sim (3u/2)^3$, while for $x_0 = 1/x_1 \sim u^4$, $z \sim u^3$. Thus, $x_0 = 1$ is the equilibrium state even at $T = 0$. There is *no* phase transition when frustrations are present.

(C) Ising gauge model.—We consider a structure, Fig. 3, on which gauge symmetry is intact. The four spins at the corners of each plaquette have a coupling $KSS'S''S'''$, $K > 0$. There are two kinds of plaquettes, drawn by thick and thin bonds. The thick plaquette at the origin $(m = 0)$ has two thin plaquettes on each of the four sides. Each of these eight thin plaquettes are connected to a thick plaquette at $m = 1$ along the "outer" side. Each of these thick plaquettes are now connected with six thin plaquettes on three sides only and

FIG. 2. A cactus on which frustration cannot be removed.
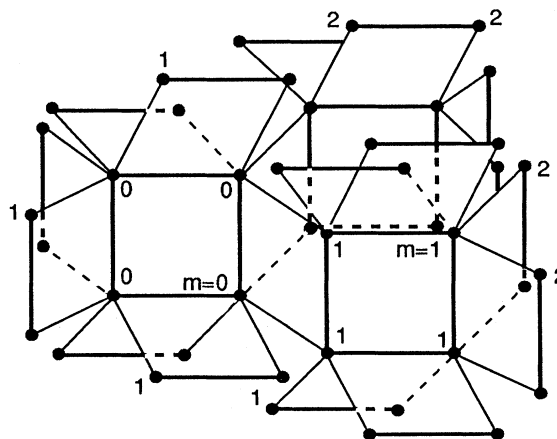

FIG. 3. A recursive lattice on which gauge symmetry is present.

so on. Since $(m + 1)$-generation sites are connected with m-generation sites pairwise, we construct $Z_m(S, S')$ for each pair. From symmetry, $Z_m(1, 1) = Z_m(-1, -1) = B_m$ and $Z_m(1, -1) = Z_m(-1, 1) = B_m x_m$. Because of these symmetries, the magnetization is *always* zero. This is consistent with the Wegner-Elitzur theorem [7], according to which the magnetization must be identically zero. The RR's are

$$B_m = 2B_{m+1}^6 f(x_{m+1}), \quad x_m = g(x_{m+1})/f(x_{m+1}),$$

where $f(x) = u + x^2(1 + 2/a) + x^4(2 + u) + x^6 = x^6 g(1/x)$ and $u = e^{2K}$. The PF $Z_0 = B_0^8 y(x_0)$ with $y(x) = 2\sqrt{u}[1 + 2x^4(1 + 2/u) + x^8]$. The free energy ω_B per plaquette is $\omega_B = (1/11) \ln[Z_0(x_0)/Z_1^6(x_1)]$, with $x = x_0 = x_1$ as the FP of the EOS, i.e., of x_m-RR. The solution $x_0 = x_1 = 1$ is always a FP. To see if there are other FP's of the EOS, we focus on $u \to \infty$. Here, $x \to u$ and $x \to 1/u$ are two other solutions. The free energy $\omega_B(1) = K + (1/11) \ln 2$ and $\omega_B(u) = \omega_B(1/u) = K + (3/11) \ln 2$ in this limit. Hence, $x = u$ or $x = 1/u$ is the equilibrium state as $u \to \infty$ and a phase transition from $x = 1$ to either of these states must occur at some finite u.

(D) Potts model.—We briefly discuss this model in the absence of any field. The reduced Hamiltonian is $\mathcal{H} = K \sum \delta_{\sigma\sigma'}$ with sum over nn spins; $\sigma = 0, 1, 2, \ldots, s$ is an $s + 1$ state Potts spin and $K > 0$. We consider the tree in Fig. 1 with $q = 3$, and set $Z_m(0) = B_m x_m$, $Z_m(1) = Z_m(2) = \cdots = Z_m(s) = B_m$, and $u = \exp K$. The RR's are

$$B_m = B_{m+1}^2 f(x_{m+1}), \quad x_m = g(x_{m+1})/f(x_{m+1}),$$

with $f(x) = x^2 + u + s - 1$ and $g(x) = ux^2 + s$. The PF $Z_0 = B_0^3 y(x_0)$, $y(x) = x^3 + s$. The free energy per bond is $\omega_B = (\frac{1}{3}) \ln f^3(x)/y$, where x is a FP of the x_m-RR, which has $x = 1$ as always a solution. The other two solutions are given by $x^2 - (u - 1)x + s = 0$. It is easy to show that there is a first order transition for $s > 1$ from $x = 1$ to $x = x_c = \rho^2 = s^{2/3}$ at $u = u_c = 1 + \rho + \rho^2$. The free energy $\omega_B(x = 1) = \omega_B(x = x_c) = (\frac{1}{3}) \ln(1 + \rho + \rho^2 + \rho^3)^3/(s + 1)$. This is consistent with the conclusion in Ref. [10].

For $s = 1$, $x_c = 1$ and the transition becomes continuous at $u_c = 3$. For $s < 1$, the situation changes. In particular, for $s = 0$, there are always three solutions $x = 0$, $x = 1$, and $x = u - 1$. However, $x = 0$ has *unbounded* free energy and must be discarded as unphysical. The other two solutions have *identical* free energy $\omega = \ln u$. Only if one applies a magnetic field H along $\sigma = 0$ state one finds that, for $u > 2$, $x = u - 1$ has a *higher* free energy than that for $x = 1$, i.e., there is a phase transition at $u = u_c = 2$, $H = 0$ with $x = u - 1$ as $H \to 0^+$ for $u > u_c$. However, at $H = 0$, this state has the *same* free energy as $x = 1$. Presumably, this unusual behavior of the Potts model for $s = 0$ is responsible for making percolation so different from usual thermal transitions.

(E) Polymers.—We consider the simplest branched polymer problem with H as the end-point activity, K as the

bond activity, and w as the trifunctional activity. (As $w \to 0$, we obtain linear polymers.) The problem is solved [8] on a cactus (Fig. 2), where only two triangles meet at a site, by relating it to a general Ising model on the tree in Fig. 1, $q = 3$. However, the Ising spins are now on bonds rather than on sites in Fig. 1. Thus, these spins form a cactus shown by thin lines in Fig. 1. A polymer bond on the original tree is said to be present if the corresponding Ising spin is in the $S = 1$ state; otherwise, the bond it absent; see Ref. [8] for more details. The RR's are similar to those in example (D) except that $f(x) = 1 + 2H\sqrt{K}x + Kx^2$ and $g(x) = \sqrt{K}(H + 2\sqrt{K}x + wKx^2)$. The PF $Z_0 = B_0^2 y(x)$, $y(x) = x^2 + 1$. Thus, the free energy per bond is given by $(\frac{1}{3}) \ln f^2(x)/(1 + x^2)$, where x is the FP of the EOS. The same free energy is obtained by integrating the equation of state as shown elsewhere [12]. We can similarly calculate the free energy for self-avoiding manifolds [13] on a recursive lattice. We will not do that here.

In summary, we have shown that calculations on Bethe or Bethe-like lattices are more reliable than conventional mean-field calculations are. We have also given an elegant and direct method for calculating the bulk free energy at the FP of the RR. This free energy must satisfy all the requirements of equilibrium thermodynamics.

The advantage of Bethe or similar recursive lattice should be apparent. By a proper choice of these lattices, it is possible to satisfy frustrations, gauge symmetries, etc., which are usually lost in conventional mean-field calculations, because of the lack of correlations. These correlations are present on Bethe lattices, even though very weak and ensure that we obtain realistic results.

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