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The large-N limit of the discrete cubic and chiral cubic models

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Abstract. The mean-field theory of the discrete cubic and chiral cubic systems is shown to be exact in the $N \to \infty$ limit.

1. Introduction

In 1974 Mittag and Stephen conjectured that the mean-field theory of the N-state Potts model is exact in the limit $N \to \infty$. This conjecture was proved by Pearce and Griffiths (1980). Here we will show that the large-N limit of the discrete cubic and chiral cubic models is mean field too, thus proving the conjecture of Badke *et al* (1985). The proof of this statement for the discrete cubic model is, except for some minor differences, the same as that given by Pearce and Griffiths for the N-state Potts model. Nevertheless we will give the proof explicitly, since we will use the solution to show that the large-N limit of the chiral cubic model is mean field, too.

The rest of this section is devoted to a precise statement of the results. In §§ 2 and 3 we obtain upper and lower bounds on the free energy of the discrete cubic model. In §§ 4 and 5 the same is done for the chiral cubic model.

The Hamiltonian of the discrete cubic model is (Nienhuis *et al* 1983 and references therein)

$$H = -\tfrac{1}{2} \sum_{i,j \in \Lambda} [K_{1_{ij}}(-1)^{\alpha_i - \alpha_j}\delta(\beta_i - \beta_j) + K_{2_{ij}}\delta(\beta_i - \beta_j)] + h_1 \sum_{i \in \Lambda} (-1)^{\alpha_i}\delta(\beta_i) + h_2 \sum_{i \in \Lambda} \delta(\beta_i) \tag{1}$$

where the vectors i and j label the sites of a regular infinite lattice $\mathscr{L}$, Λ is a finite subset of $\mathscr{L}$, and the $2N$ possible states at each site are given by $\alpha_i = 0, 1$ and $\beta_i = 0, 1, \ldots, N-1$. The partition function is

$$Z_\Lambda(\beta) = \sum_{\{\alpha_i, \beta_i\}} \exp(-\beta H) \tag{2}$$

where $\beta = 1/kT$. The free energy per site $\psi(\beta)$ in the thermodynamic limit is given by

$$-\beta\psi(\beta) = \lim_{\Lambda \to \mathscr{L}} |\Lambda|^{-1} \ln Z_\Lambda(\beta) \tag{3}$$

where $|\Lambda|$ is the number of sites in Λ.

We will assume that the interactions are ferromagnetic and translationally invariant,

$$K_{a_{ij}} = K_a(i-j) \geqslant 0 \qquad (a = 1, 2) \tag{4}$$

with sufficiently rapid decay

$$K_a = \sum_{j \in \mathscr{L}} K_{a_{ij}} < \infty. \tag{5}$$

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Under these conditions (see Ruelle 1969) the limiting free energy (3) exists and does not depend on the choice of the boundary conditions. We will prove the following.

Theorem 1. Let $\psi(\beta)$ be the free energy (3) for the discrete cubic system (1), with interactions satisfying (4) and (5) and h_1, $h_2 \geq 0$. Then in the large-N limit

$$\lim_{N\to\infty} \psi(\beta \ln N) = \lim_{N\to\infty} \psi_{\mathrm{MF}}(\beta \ln N) = \psi_\infty(\beta) \tag{6}$$

where $\psi_{\mathrm{MF}}(\beta)$ is the mean-field free energy and

$$\psi_\infty(\beta) = \begin{cases} -\beta^{-1}, & \beta(\frac{1}{2}K_1 + h_1 + \frac{1}{2}K_2 + h_2) \leq 1, \\ -(\frac{1}{2}K_1 + h_1 + \frac{1}{2}K_2 + h_2), & \beta(\frac{1}{2}K_1 + h_1 + \frac{1}{2}K_2 + h_2) > 1. \end{cases} \tag{7}$$

The factor $\ln N$ which appears in the argument of ψ in (6) is essential in order to obtain a non-trivial result in the limit $N \to \infty$.

The Hamiltonian of the chiral cubic model is (Badke *et al* 1985)

$$H = -\tfrac{1}{2} \sum_{i,j\in\Lambda} \sum_{\mu} J_{\mu_{ij}} \chi_\mu(g_i g_j^{-1}) - \sum_{i\in\Lambda} \sum_{\mu} h_\mu \chi_\mu(g_i), \qquad g \in \mathrm{W}_N, \tag{8}$$

where W_N is the group of all $N \times N$ orthogonal matrices with integer elements and χ_μ is the character function corresponding to the irreducible representation μ of W_N. In the following we will restrict our investigations to the vector representation, since it is the smallest faithful irreducible representation of W_N. Hence, taking χ for the character of the vector representation,

$$H = -\tfrac{1}{2} \sum_{i,j\in\Lambda} J_{ij} N^{-1} \chi(g_i g_j^{-1}) - \sum_{i\in\Lambda} h N^{-1} \chi(g_i) \tag{9}$$

where the factor N^{-1} has been introduced for convenience. The partition function is

$$Z_\Lambda(\beta) = \sum_{\{g_i\}} \exp(-\beta H) \tag{10}$$

and the free energy per site is

$$\phi(\beta) = -\beta^{-1} \lim_{\Lambda\to\mathscr{L}} |\Lambda|^{-1} \ln Z_\Lambda(\beta). \tag{11}$$

We will prove the following.

Theorem 2. Let $\phi(\beta)$ be the free energy (11) for the chiral cubic model (9), with interactions satisfying

$$J_{ij} = J(i-j) \geq 0 \qquad \text{and} \qquad J = \sum_{j\in\mathscr{L}} J_{ij} < \infty \tag{12}$$

and $h \geq 0$. Then in the large-N limit

$$\lim_{N\to\infty} \phi(\beta N \ln N) = \lim_{N\to\infty} \phi_{\mathrm{MF}}(\beta N \ln N) = \phi_\infty(\beta) \tag{13}$$

where $\phi_{\mathrm{MF}}(\beta)$ is the mean-field free energy and

$$\phi_\infty(\beta) = \begin{cases} -\beta^{-1}, & \beta(\frac{1}{2}J + h) \leq 1, \\ -(\frac{1}{2}J + h), & \beta(\frac{1}{2}J + h) > 1. \end{cases} \tag{14}$$

2. The mean-field free energy of the discrete cubic model

Let H be defined by (1) and impose periodic boundary conditions so that

$$K_a^\Lambda = \sum_{j\in\Lambda} K_{a_{ij}} \to K_a \qquad \text{as } \Lambda \to \mathscr{L} (a=1,2) \tag{15}$$

and K_a^Λ do not depend on i.

For any other Hamiltonian H_0 the following inequality holds:

$$\begin{aligned}|\Lambda|^{-1} \ln Z_\Lambda(\beta) &= |\Lambda|^{-1}(\ln Z_{0_\Lambda}(\beta) + \ln\langle \exp[-\beta(H-H_0)]\rangle_0) \\ &\geqslant |\Lambda|^{-1}(\ln Z_{0_\Lambda}(\beta) - \beta\langle H - H_0\rangle_0)\end{aligned} \tag{16}$$

where $Z_{0_\Lambda}(\beta) = \Sigma \exp(-\beta H_0)$, $\langle X\rangle_0 = Z_{0_\Lambda}^{-1} \Sigma\, X \exp(-\beta H_0)$ and Z_Λ is given by (2). The inequality follows from the convexity of the exponential function. In order to calculate the mean-field free energy one has to use the RHS of (16) choosing H_0 as follows (see, for example, Ditzian *et al* 1980):

$$H_0 = -\sum_{i\in\Lambda}\left(\sum_{l=0}^{N-1} [(-1)^{\alpha_i}\delta(\beta_i - l)g_l^i + \delta(\beta_i - l)f_l^i] + h_1(-1)^{\alpha_i}\delta(\beta_i) + h_2\delta(\beta_i)\right) \tag{17}$$

where

$$g_l^i = \sum_{j\in\Lambda} K_{1_{ij}}\langle(-1)^{\alpha_j}\delta(\beta_j - l)\rangle_0, \qquad f_l^i = \sum_{j\in\Lambda} K_{2_{ij}}\langle\delta(\beta_j - l)\rangle_0. \tag{18}$$

(The factor of 2 is due to the double counting in (1). We have used the identity $\delta(\beta_i - \beta_j) = \Sigma_{l=0}^{N-1}\, \delta(\beta_i - l)\, \delta(\beta_j - l)$.) Due to translation invariance and the symmetry of the interactions, we have

$$g_l^i = \begin{cases} K_1^\Lambda p, & l=0, \\ 0, & l\neq 0, \end{cases} \qquad \text{and} \qquad f_l^i = \begin{cases} K_2^\Lambda \bar{q}, & l=0, \\ K_2^\Lambda \dfrac{1-\bar{q}}{N-1}, & l\neq 0, \end{cases} \tag{19}$$

where the values of p and $\bar{q}$ maximise the RHS of (16) with $0 \leqslant \bar{q} \leqslant 1$ and $|p| \leqslant \bar{q}$. For convenience, we will choose the order parameter $q = \bar{q} - N^{-1}$ instead of $\bar{q}$. If we now evaluate the RHS of (16), maximise it with respect to p and q and take the thermodynamic limit we obtain

$$\begin{aligned}-\beta\psi(\beta) &\geqslant -\beta\psi_{\mathrm{MF}}(\beta) \\ &= \max_{(p,q)}\left\{\ln\left[2\cosh[\beta(pK_1 + h_1)]\exp[\beta(qK_2 + h_2)]\right.\right. \\ &\quad \left.\left. + 2(N-1)\exp\left(-\beta\frac{K_2 q}{N-1}\right)\right] + \frac{\beta K_2}{2N} - \frac{\beta}{2}\left(K_1 p^2 + K_2 q^2 \frac{N}{N-1}\right)\right\}.\end{aligned} \tag{20}$$

After replacing β by $\beta \ln N$ one obtains in the limit $N\to\infty$

$$\lim_{N\to\infty} \psi(\beta \ln N) \leqslant \lim_{N\to\infty} \psi_{\mathrm{MF}}(\beta \ln N) = \psi_\infty(\beta) \tag{21}$$

where $\psi_\infty(\beta)$ is given by (7).

3. A lower bound on ψ

For the sake of completeness, we will copy in this section the bound of Pearce and

Griffiths (1980), adapted to the special properties of the discrete cubic model†. To obtain an upper bound on the partition function and thus a lower bound on the free energy ψ it is convenient to employ a different set of boundary conditions on the finite subset Λ, and to restrict the interactions to finite range. Namely, we will assume that $\alpha_i = \beta_i = 0$ for all sites i not in Λ, and write

$$H^R = -\tfrac{1}{2} \sum_{i\in\Lambda} \sum_{j\in\mathscr{L}} [K^R_{1_{ij}}(-1)^{\alpha_i-\alpha_j}\delta(\beta_i-\beta_j) + K^R_{2_{ij}}\delta(\beta_i-\beta_j)] - h_1 \sum_{i\in\Lambda} (-1)^{\alpha_i}\delta(\beta_i) - h_2 \sum_{i\in\Lambda} \delta(\beta_i) \tag{22}$$

where, for a fixed distance R, we define the truncated interactions

$$K^R_{a_{ij}} = \begin{cases} K_{a_{ij}}, & |i-j| < R \\ 0, & |i-j| \geq R \end{cases} \qquad (a = 1, 2). \tag{23}$$

The minimum value of H^R,

$$\bar{H} = -|\Lambda|(\tfrac{1}{2}K^R_1 + \tfrac{1}{2}K^R_2 + h_1 + h_2), \tag{24}$$

occurs when all α_i and β_i are equal to zero. The basic inequality $H^R \geq \bar{H}$ can now be improved by using graphical methods. With every configuration of the system, i.e. with every choice of the α_i and β_i, $i \in \Lambda$, associate a graph G whose vertices are the sites at which $\beta_i \neq 0$, with edges connecting the vertices provided $\beta_i = \beta_j (\neq 0)$ and $|i-j| < R$. Let μ be the number of connected components in G. The number of configurations associated with the same graph G cannot exceed $2^{|\Lambda|}\,(N-1)^{\mu}$, since $\alpha_i = 0, 1$ and the β_i are identical in each component. The number of distinct graphs is itself bounded by $2^{|\Lambda|Z/2}$, where Z is the number of sites on the lattice within a distance R of a particular site. This estimate holds because a graph is determined by specifying all its edges, and there are at most $\frac{1}{2}|\Lambda|Z$ possible edges connecting pairs of sites in Λ separated by a distance less than R.

We now assert that

$$H^R \geq \bar{H} + \mu(\tfrac{1}{2}K^R_1 + \tfrac{1}{2}K^R_2 + h_1 + h_2) \tag{25}$$

where μ is defined for a choice of β_i in the manner described above. To see this, note first that the number of sites with $\beta_i \neq 0$ is at least μ; this accounts for the $\mu(h_1 + h_2)$ term in (25). Next, note that for any connected component C in the graph G and for any vector r connecting two sites in $\mathscr{L}$, there will always be some site i in C such that $i + r$ is not in C. Now if $i \in C$ and $(i + r) \notin C$, then $\beta_i \neq \beta_{i+r}$ provided $|r| < R$, and thus the corresponding term in (22) is zero, rather than $-(\frac{1}{2}K^R_1(r) + \frac{1}{2}K^R_2(r))$ as it is in the case where all α_i and β_i are zero. Since for each component and for each r with $|r| < R$ we can identify a corresponding increment in H^R over $\bar{H}$, we have established the validity of the $\mu(\frac{1}{2}K^R_1 + \frac{1}{2}K^R_2)$ term in (25).

Collecting terms we have

$$\begin{aligned} Z^R_\Lambda(\beta) &\leq 2^{Z|\Lambda|/2} \exp(-\beta\bar{H}) 2^{|\Lambda|} \sum_{\mu=0}^{|\Lambda|} \{N \exp[-\beta(\tfrac{1}{2}K^R_1 + \tfrac{1}{2}K^R_2 + h_1 + h_2)]\}^{\mu} \\ &\leq 2^{(z/2+1)|\Lambda|} \exp(-\beta\bar{H}) \{1 + N \exp[-\beta(\tfrac{1}{2}K^R_1 + \tfrac{1}{2}K^R_2 + h_1 + h_2)]\}^{|\Lambda|}. \end{aligned} \tag{26}$$

† It is also possible to obtain a lower bound on ψ with algebraic bounds along the lines of Pearce (1984) instead of by the graphical methods used here. Doing this one obtains

$$\psi(\beta \ln N) \rightleftharpoons -(\beta \ln N)^{-1}[\![\ln 2 + \ln\{\exp[\beta \ln N(\tfrac{1}{2}K_1 + \tfrac{1}{2}K_2 + h_1 + h_2)] + N - 1\}]\!] \xrightarrow[N\to\infty]{} \psi_\infty(\beta).$$

Using (3) and (24) it follows that

$$\psi^R(\beta) \geq -\beta^{-1}(1+Z/2)\ln 2 - \beta^{-1}\ln\{N+\exp[\beta(\tfrac{1}{2}K_1^R+\tfrac{1}{2}K_2^R+h_1+h_2)]\}. \tag{27}$$

After replacing β by $\beta \ln N$ in this expression, one obtains

$$\lim_{N\to\infty} \psi^R(\beta \ln N) \geq \psi^R_\infty(\beta) \tag{28}$$

where $\psi^R_\infty(\beta)$ is given by (7) with K_a^R in place of K_a $(a=1,2)$. Combining (21) and (28), theorem 1 is proved for interactions of strictly finite range.

When the interactions are not of strictly finite range, but (5) is satisfied, our arguments yield (7) provided the limit $R\to\infty$ is taken after the limit $N\to\infty$, since

$$K_a^R = \sum_{r:\,|r|<R} K_a(r) \to K_a \qquad \text{as } R\to\infty. \tag{29}$$

Now standard arguments (Ruelle 1969) can be used to show that for any finite N and β,

$$|\psi-\psi^R| \leq \sum_{r:\,|r|\geq R} (K_1(r)+K_2(r)) \tag{30}$$

so that in view of (29) the convergence of ψ^R to ψ as $R\to\infty$ is uniform in N and β, which means that the limits $N\to\infty$ and $R\to\infty$ are interchangeable. Thus theorem 1 is proved.

4. The mean-field free energy of the chiral cubic model

Let H be defined by (9) and impose periodic boundary conditions so that

$$J^\Lambda = \sum_{j\in\Lambda} J_{ij} \to J \qquad \text{as } \Lambda \to \mathscr{L} \tag{31}$$

and J^Λ does not depend on i.

Here again we will use the inequality

$$|\Lambda|^{-1}\ln Z_\Lambda(\beta) \geq |\Lambda|^{-1}(\ln Z_{0_\Lambda}(\beta) - \beta\langle H-H_0\rangle_0) \tag{32}$$

where now Z is given by (10), $Z_0=\Sigma\exp(-\beta H_0)$ and H_0 has to be chosen as follows in order to get the mean-field theory:

$$H_0 = -\sum_{i\in\Lambda} N^{-1}[\chi(g_iA_i^{\mathrm{T}})+h\chi(g_i)] \tag{33}$$

where A_i are $N\times N$ matrices given by

$$(A_i)_{k,l} = \sum_{j\in\Lambda} J_{ij}\langle (g_j)_{k,l}\rangle_0. \tag{34}$$

(Notice that $\chi(g_ig_j^{-1})=\chi(g_ig_j^{\mathrm{T}})=\Sigma_{k,l=1}^N (g_i)_{k,l}\ (g_j)_{k,l}$.)

Due to the symmetry of the interactions, we have

$$(A_i)_{k,l} = \alpha J^\Lambda \delta_{k,l} \tag{35}$$

where the value of α maximises the RHS of (32) with $0\leq\alpha\leq 1$. If we now evaluate the RHS of (32), maximise it with respect to α and take the thermodynamic limit we obtain

$$\phi(\beta) \leq \phi_{\mathrm{MF}}(\beta) = -\beta^{-1}\max_{0\leq\alpha\leq1}\left[-\tfrac{1}{2}\beta J\alpha^2 + \ln\left(\sum_{g\in W_N}\exp[\beta(\alpha J+h)N^{-1}\chi(g)]\right)\right]. \tag{36}$$

After replacing β by $\beta N \ln N$ in (36) one obtains in the limit $N \to \infty$

$$\lim_{N\to\infty} \phi(\beta N \ln N) \leqslant \lim_{N\to\infty} \phi_{\mathrm{MF}}(\beta N \ln N) = \phi_\infty(\beta) \tag{37}$$

where $\phi_\infty(\beta)$ is given by (14).

To see this, let $G(N, k)$ be the number of group elements of W_N with $\chi(g) = k$. Clearly $\Sigma_{k=-N}^{N} G(N, k) = 2^N N!$. For $k \geqslant 0$ Baake (1984) gives the formula

$$G(N, k) = 2^{N-k} N! \sum_{\nu=0}^{[(N-K)/2]} [2^{2\nu} \nu! (\nu+k)!]^{-1} \sum_{\mu=0}^{N-k-2\nu} (-1)^\mu/\mu!,$$

$$G(N, -k) = G(N, k). \tag{38}$$

Having this formula one can easily show that

$$\tfrac{1}{4} G(N, k-1) \leqslant k G(N, k) \leqslant G(N, k-1) \qquad \text{for } 1 \leqslant k \leqslant N-2. \tag{39}$$

Let

$$f(N; \gamma) = (N \ln N)^{-1} \ln\left(\sum_{k=-N}^{N} G(N, k) N^{\gamma k} \right). \tag{40}$$

Using (39) one can show that

$$\lim_{N\to\infty} f(N; \gamma) = \begin{cases} 1, & \gamma \leqslant 1, \\ \gamma, & \gamma > 1, \end{cases} \qquad \text{and} \qquad \lim_{N\to\infty} \frac{\partial f(N; \gamma)}{\partial \gamma} = \begin{cases} 0, & \gamma < 1, \\ 1, & \gamma > 1. \end{cases} \tag{41}$$

Now from (36) one gets

$$\phi_{\mathrm{MF}}(\beta N \ln N) = \min_{0 \leqslant \alpha \leqslant 1} \{ -\beta^{-1} f[N; \beta(\alpha J + h)] + \tfrac{1}{2} J \alpha^2 \} \tag{42}$$

and taking the limit $N \to \infty$ one obtains (37).

5. A lower bound on ϕ

To get an upper bound on the partition function of the chiral cubic model, we will first write the Hamiltonian (9) in a more convenient form. Every group element $g \in \mathrm{W}_N$ (see Baake 1984) can be labelled by an N-component vector $\boldsymbol{a}$, with components equal to zero or one, and a permutation π of N objects; so $g = (\boldsymbol{a}, \pi)$. In this notation we have

$$\begin{aligned} \chi(g) &= \sum_{\nu=1}^{N} (-1)^{a_\nu} \delta(\pi(\nu) - \nu), \\ \chi(g_i g_j^{-1}) &= \sum_{\nu=1}^{N} (-1)^{a_i^\nu - a_j^\nu} \delta(\pi_i(\nu) - \pi_j(\nu)). \end{aligned} \tag{43}$$

Hence the Hamiltonian (9) reads

$$H = \sum_{\nu=1}^{N} N^{-1} \left(\sum_{i,j \in \Lambda} \tfrac{1}{2} J_{ij} (-1)^{a_i^\nu - a_j^\nu} \delta(\pi_i(\nu) - \pi_j(\nu)) + h \sum_{i \in \Lambda} (-1)^{a_i^\nu} \delta(\pi_i(\nu) - \nu) \right). \tag{44}$$

Let

$$\hat{H}_\nu = -\tfrac{1}{2} \sum_{i,j \in \Lambda} J_{ij} (-1)^{a_i^\nu - a_j^\nu} \delta(b_{i_\nu} - b_{j_\nu}) - h \sum_{i \in \Lambda} (-1)^{a_i^\nu} \delta(b_{i_\nu} - \nu) \tag{45}$$

where $\nu = 1, \ldots, N$ and $b_{i_\nu} = 1, \ldots, N$. If $\hat{H} = N^{-1} \sum_{\nu=1}^{N} \hat{H}_\nu$ and $\boldsymbol{b}_i = (b_{i_1}, \ldots, b_{i_N})$ then one has for the partition function of the chiral cubic model (44)

$$Z_\Lambda(\beta) = \sum_{\{\boldsymbol{a}_i, \pi_i\}} \exp(-\beta H) \le \sum_{\{\boldsymbol{a}_i, \boldsymbol{b}_i\}} \exp(-\beta \hat{H})$$

$$= \prod_{\nu=1}^{N} \left(\sum_{\{\boldsymbol{a}_i^\nu, \boldsymbol{b}_i^\nu\}} \exp(-\beta N^{-1} \hat{H}_\nu) \right) = [\tilde{Z}_\Lambda(N^{-1}\beta)]^N \tag{46}$$

where $\tilde{Z}_\Lambda(\beta)$ is the partition function of the discrete cubic model (1) with $K_{1_{ij}} = J_{ij}$, $h_1 = h$ and $K_{2_{ij}} = h_2 = 0$.

So we get for the free energy

$$\phi(\beta) \ge \tilde{\psi}(N^{-1}\beta). \tag{47}$$

Thus from theorem 1 and (14)

$$\lim_{N\to\infty} \phi(\beta N \ln N) \ge \lim_{N\to\infty} \tilde{\psi}(\beta \ln N) = \phi_\infty(\beta). \tag{48}$$

With (37) and (48) the proof of theorem 2 is complete.

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