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The infinite-coordination limit for classical spin systems on irregular lattices

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Abstract. For n-vector classical spin systems with coordination numbers q_i and average coordination q it is proved that the free energy is given, in the high density limit, by the Curie-Weiss expression, provided that the average of the relative deviation $|1-q_i/q|$ over the system vanishes in the same limit. Some factors concerning the surface influence on the free energy are then treated.

1. Introduction

The classical Curie-Weiss theory, which provides an insight into the understanding of phase transitions in ferromagnetic systems, has been established rigorously using various spin models.

Molecular fields can be obtained in the long range limit of Kac-type potentials

$$\rho_{ij} = \gamma^d \rho(\gamma|\boldsymbol{i}-\boldsymbol{j}|)$$

(Thompson and Silver 1973, Pearce and Thompson 1975).

In some particular cases, Curie-Weiss theory has been established by considering a short range potential on spin lattices in the high density limit (infinite coordination limit). The high density limit for Ising spin models was obtained by Thompson (1974). The method proposed is a graph-theoretical one, and it works on any lattice with coordination number q. Because generalisation to other than Ising spin models is difficult, an algebraic method, known as the coalescing bound method (or TS method) developed by Thompson and Silver (1973), was applied by Pearce and Thompson (1978) for the exact computation of the free energy for n-vector models on regular lattices. In its original form, the method could not avoid diagonalisation of a particular cyclic matrix (corresponding to regular lattices of increasing coordination).

In this paper some technical amendments are made in order to generalise the result obtained by Pearce and Thompson (1978) to any n-vector classical spin system in the $q\to\infty$ limit, provided that the deviation from the average coordination becomes negligible (in a sense specified below) in this limit. In § 2 it is proved that, for such systems, the Curie-Weiss expression for the free energy is valid in the high density limit. In § 3 this result is applied to the study of the surface influence on the free energy of bounded lattices and of highly anisotropic spin systems on two particular models.

Consider the Hamiltonian

$$\mathcal{H}^n = -(2q)^{-1} J \sum_{i,j=1}^{N} A_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \boldsymbol{H} \cdot \sum_{i=1}^{N} \boldsymbol{S}_i \tag{1.1}$$

where the symmetric matrix A is given by

$$A_{ij} = \begin{cases} 1 & \text{for interacting spins} \\ 0 & \text{otherwise} \end{cases} \tag{1.2}$$

and

$$q = N^{-1} \sum_{i=1}^{N} q_i \qquad \text{with} \qquad q_i = \sum_{j=1}^{N} A_{ij}. \tag{1.3}$$

The following constraint is imposed on the matrix A:

$$\lim_{N,q\to\infty} \varepsilon_{N,q} = 0 \tag{1.4}$$

with

$$\varepsilon_{N,q} = (Nq)^{-1} \sum_{i=1}^{N} |q_i - q| \tag{1.5}$$

i.e. the deviation from the average coordination must be negligible.

The free energy, $\psi^n(\beta, \boldsymbol{H}; q)$, is defined as

$$\psi^n(\beta, \boldsymbol{H}; q) = \lim_{N\to\infty} \psi^n_N(\beta, \boldsymbol{H}; q) \tag{1.6}$$

with

$$-\beta\psi^n_N(\beta, \boldsymbol{H}; q) = N^{-1} \log Z^n_N(\beta, \boldsymbol{H}; q) \tag{1.7}$$

$$Z^n_N(\beta, \boldsymbol{H}; q) = A_n^{-N} \int \ldots \int_{\|\boldsymbol{S}_i\| = n^{1/2}} \mathrm{d}^N \boldsymbol{S} \exp(-\beta \mathcal{H}^n) \tag{1.8}$$

and

$$A_n = 2\pi^{n/2} n^{(n-1)/2} / \Gamma(n/2). \tag{1.9}$$

The main result is the following theorem, proved in § 2.

Theorem. For the n-vector spin systems specified by (1.1)-(1.9), the limiting free energy is given by

$$\psi^n(\beta, \boldsymbol{H}) = \lim_{q\to\infty} \psi^n(\beta, \boldsymbol{H}; q) = \min_x [\tfrac{1}{2} n J x^2 - \beta^{-1} \log \mathcal{I}_n(\beta J x + \beta H)] \tag{1.10}$$

with $H = n^{-1/2} \|\boldsymbol{H}\|$ and

$$\mathcal{I}_n(x) = \Gamma(n/2) I_{n/2-1}(nx) / (\tfrac{1}{2} n x)^{n/2-1}.$$

I_μ is the modified Bessel function of order μ.

2. Proof of the theorem

In order to obtain the limiting free energy (1.10), we shall follow the general scheme of the TS method.

The upper bound of the free energy (1.6) is given by (1.10). This fact is easily proved using Jensen's inequality, relation (1.4) and direct computation of the remaining integrals. For details see, for example, Thompson and Silver (1973), in which these manipulations are done for a similar case.

The lower bound is more easily obtained if we compute it for an equivalent matrix of interaction—i.e. leading to the same limiting free energy—having the maximum eigenvalue close to its medium coordination. One way of obtaining such a matrix, A', together with the sufficient condition of equivalence which applies to this case, is given in appendix 1. The matrix obtained there has, in addition, the following properties (see relations (A1.7) and (A1.8)):

$$\max_i q_i' \leqslant q$$

and

$$\lim_{q\to\infty} q'/q = 1.$$

The estimation of the eigenvalues of A' is done by the following lemma.

Lemma. The eigenvalues a_i of a matrix of type (1.2) are evaluated by

$$-q_M \leqslant a_i \leqslant q_M \qquad i = 1, \ldots, N \tag{2.1}$$

where

$$q_M = \max_i q_i.$$

Proof. The min-max principle is used. Noting that the elements A_{ij} are non-negative, (2.1) follows directly from

$$\left| \sum_{i,j=1}^{N} A_{ij} x_i x_j \right| \leqslant \sum_{i,j=1}^{N} A_{ij} x_i^2 = \sum_{i=1}^{N} x_i^2 \sum_{j=1}^{N} A_{ij} \leqslant q_M$$

(with $\Sigma_{i=1}^{N} x_i^2 = 1$).

We see now from (A1.8) and (2.1) that the eigenvalues of A' obey the inequality

$$|a_i'| \leqslant q. \tag{2.2}$$

Following the general ideas of Pearce and Thompson (1978), set

$$|A'| = S \operatorname{diag}\{|a_i'|\} S^{-1} \tag{2.3}$$

with S chosen such that

$$A' = S \operatorname{diag}\{a_i'\} S^{-1} \tag{2.4}$$

and

$$qK_{ij} = |A'|_{ij} + q\varepsilon\delta_{ij} \qquad (\varepsilon > 0). \tag{2.5}$$

Since the matrix $qK - A'$ is positive definite, the following inequality holds for the partition function related to A'

$$Z'^{n}_{N}(\beta, \boldsymbol{H}; q') \leqslant A_n^{-N} \int_{\|\boldsymbol{S}_i\|=n^{1/2}} \cdots \int \mathrm{d}^N\boldsymbol{S} \exp\left(\tfrac{1}{2}\nu' \sum_{i,j} K_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \beta\boldsymbol{H} \cdot \sum_i \boldsymbol{S}_i\right)$$

$$(\nu' = \beta J',\ J' = Jq(q')^{-1}). \tag{2.6}$$

Using a standard identity (see Pearce and Thompson 1975), we can rewrite (2.6) in the following form:

$$Z'^{n}_{N}(\beta, \boldsymbol{H}; q') \leqslant (2\pi)^{-Nn/2} A_n^{-N} (\det K/\nu')^{-n/2} \int_{-\infty}^{\infty} \cdots \int \mathrm{d}^N\boldsymbol{x}$$

$$\times \exp\left(-\tfrac{1}{2}\nu' \sum_{i,j} K_{ij}^{-1} \boldsymbol{x}_i \cdot \boldsymbol{x}_j\right) \int_{\|\boldsymbol{S}_i\|=n^{1/2}} \cdots \int \mathrm{d}^N\boldsymbol{S} \exp\left(\sum_i \nu' \boldsymbol{x}_i + \beta\boldsymbol{H}\right) \cdot \boldsymbol{S}_i \tag{2.7}$$

$$= (2\pi)^{-Nn/2} (\det K/\nu')^{-n/2} \int_{-\infty}^{\infty} \cdots \int \mathrm{d}^N\boldsymbol{x} \exp\left(-\tfrac{1}{2}\nu' \sum_{i,j} (K_{ij}^{-1} - z^{-1}\delta_{ij}) \boldsymbol{x}_i \cdot \boldsymbol{x}_j\right)$$

$$\times \prod_i \exp[-\tfrac{1}{2}\nu' z^{-1} \|\boldsymbol{x}_i\|^2 + \log \mathcal{I}_n(n^{-1/2} \|\nu' \boldsymbol{x}_i + \beta\boldsymbol{H}\|)] \tag{2.8}$$

where the function $\mathcal{I}_n$ is given by (1.11), $z = \alpha(1+\varepsilon)$, $\alpha > 1$, keeps the matrix $\{K_{ij}^{-1} - z^{-1}\delta_{ij}\}$ positive definite.

Maximisation of each term of the product in (2.8) and computation of the remaining Gaussian integrals leads to

$$\psi^n_N(\beta, \boldsymbol{H}; q) \geqslant \min_x [\tfrac{1}{2} n z^{-1} J' x^2 - \beta^{-1} \log \mathcal{I}_n(\beta J' x + \beta H)]$$

$$+ (2N)^{-1} n\beta \log[\det(I - K/z)] \qquad (x = n^{-1/2}\|\boldsymbol{x}\|). \tag{2.9}$$

Taking the limits $\varepsilon \to 0$, $N \to \infty$, $q \to \infty$ (after which $J = J'$, see (A1.7)) and $\alpha \to 1$, the proof is completed, since the error term

$$E_{N,q}(\alpha, \varepsilon) = (2N)^{-1} n\beta \log[\det(I - K/z)] \tag{2.10}$$

as shown in appendix 2, vanishes in the same limits.

As a particular case, the result of the theorem applies, of course, to any 'homogeneous' system ($q_i = q$ for all i), with short range interactions of type (1.2), independent of the type of lattice, its regularity or space dimension.

A system for which condition (1.4) is not trivially fulfilled will appear in the next section.

3. Bounded systems

We shall first apply the theorem of § 1 to evaluate the surface influence on the free energy for $d \to \infty$ models. Consider first the model of a d-dimensional bounded cubic lattice with $m > 2$ vertices in each direction (m is a constant of the problem) and a nearest-neighbour interaction of type (1.2). In view of its boundedness and absence of cyclicity conditions, this system may seem to present strong surface effects but, as will be shown, this is not the case.

As can be seen from the development of p^d in powers of $(p-2)$, the number of k-dimensional faces is

$$C_d^k 2^{d-k}. \tag{3.1}$$

Now, simple algebra shows that

$$q = 2d(1-m^{-1}) \tag{3.2}$$

and also

$$q^{-1}N^{-1}\sum_j |q_j - q| \leq d^{-1/2}m(m-2)^{-1/2} \tag{3.3}$$

so that the theorem applies to our system and the free energy is the same as if cyclicity conditions were imposed to suppress the surface. This is due to the fact that, in the infinite dimensionality limit, the number of spins situated on faces with some particular dimensions (in our case, close to $d(1-2m^{-1})$) becomes dominant, and the geometry of even bounded systems becomes insignificant. Clearly, surface effects can be revealed only if a sufficiently strong anisotropy is imposed on the system. We shall choose a system which is, in some aspects, the $d\to\infty$ analogue of the model considered by Pearce (1977). Consider the Hamiltonian

$$\mathscr{H} = -J(2q)^{-1}\sum_{i,j}\sum_{t=1}^{T} A_{ij}\boldsymbol{S}_{it}\cdot\boldsymbol{S}_{jt} - J\sum_{i}\sum_{t=1}^{T}\boldsymbol{S}_{it}\cdot\boldsymbol{S}_{it+1} - \boldsymbol{H}\cdot\sum_{i,t}\boldsymbol{S}_{it} \tag{3.4}$$

where A_{ij} is a matrix of type (1.2)-(1.5) and T is considered constant througout the problem. The n-vector partition function is given by

$$Z^n_{N,T}(\beta,\boldsymbol{H};q) = A_n^{-NT}\int_{\|\boldsymbol{S}_{it}\|=n^{1/2}}\!\!\!\cdots\int \mathrm{d}^{NT}\boldsymbol{S}\exp(-\beta\mathscr{H}) \tag{3.5}$$

with A_n given by (1.9); the other functions are defined as in § 1.

Although for this system the theorem cannot be directly applied, the computation of the free energy follows essentially the same path, so we shall only sketch it here.

In the $N\to\infty$, $q\to\infty$ limit, the free energy is given by

$$\psi^n_T(\beta,\boldsymbol{H}) = T^{-1}\min_{x_t}\left(\tfrac{1}{2}J\sum_t x_t^2 - \beta^{-1}\log U_{nT}(\nu,\boldsymbol{B}+\nu\boldsymbol{x}_1,\ldots,\boldsymbol{B}+\nu\boldsymbol{x}_T)\right) \tag{3.6}$$

with

$$U_{nT}(\nu,\boldsymbol{B}+\nu\boldsymbol{x}_1,\ldots,\boldsymbol{B}+\nu\boldsymbol{x}_T) = A_n^{-T}\int_{\|\boldsymbol{S}_t\|=n^{1/2}}\exp\bigg(\beta J\sum_t \boldsymbol{S}_t\cdot\boldsymbol{S}_{t+1}$$

$$+\beta\sum_t(\boldsymbol{H}+J\boldsymbol{x}_t)\cdot\boldsymbol{S}_t\bigg)\,\mathrm{d}^T\boldsymbol{S} \qquad (\boldsymbol{B}=\beta\boldsymbol{H},\ \nu=\beta J). \tag{3.7}$$

The existence of the absolute minimum in (3.6) is obvious from (3.7). The upper bound can again be found in the standard way. For the lower bound, the matrix $\{A_{ij}\}$

is again replaced by its equivalent $\{A'_{ij}\}$. The same construction (2.2)-(2.4) is then applied to the matrix A'. This gives

$$Z^n_{N,T}(\beta, \boldsymbol{H}; q) \leq (2\pi)^{-NTn/2}(\det K/\nu')^{-Tn/2} A_n^{-NT} \int_{-\infty}^{\infty}\!\!\dots\!\int \mathrm{d}^{NT}\boldsymbol{x}$$

$$\times \exp\left(-\tfrac{1}{2}\nu' \sum_{i,j,t} (K_{ij}^{-1} - z^{-1}\delta_{ij})\boldsymbol{x}_{it}\cdot\boldsymbol{x}_{jt}\right) \int\!\!\dots\!\int_{\|\boldsymbol{S}_{it}\|=n^{1/2}} \exp\left(-(2z)^{-1}\nu' \sum_{i,t} \boldsymbol{x}_{it}^2\right.$$

$$\left. + \nu' \sum_{i,t} \boldsymbol{S}_{it}\cdot\boldsymbol{S}_{it+1} + \sum_{i,t} (\boldsymbol{B} + \nu'\boldsymbol{x}_{it})\cdot\boldsymbol{S}_{it}\right) \mathrm{d}^{NT}\boldsymbol{S}$$

$$= (2\pi)^{-nNT/2}(\det K/\nu')^{-nT/2} \int_{-\infty}^{\infty}\!\!\dots\!\int \mathrm{d}^{NT}x$$

$$\times \exp\left(-\tfrac{1}{2}\nu' \sum_{i,j,t} (K_{ij}^{-1} - z^{-1}\delta_{ij})\boldsymbol{x}_{it}\cdot\boldsymbol{x}_{jt}\right)$$

$$\times \prod_i \exp\left(-\tfrac{1}{2}\nu' z^{-1} \sum_t \boldsymbol{x}_{it}^2 + \log U_{nT}(\nu, \boldsymbol{B} + \nu'\boldsymbol{x}_{i1}, \dots, \boldsymbol{B} + \nu'\boldsymbol{x}_{iT})\right). \tag{3.8}$$

After the maximisation of each term of the product appearing in (3.8), the same steps as used in the preceding section can be applied to (3.8) to obtain the final lower bound.

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Appendix 1

Let B and B' be two matrices for the Hamiltonian (1.1), q and q' their medium coordinations, defined through (1.3), and ψ_N^n, $\psi_N'^n$ given by (1.7).

Lemma. If B and B' are correlated so that

$$\lim_{N,q\to\infty} N^{-1}q^{-1} \sum_{i,j=1}^{N} |B_{ij} - B'_{ij}| = 0 \tag{A1.1}$$

then

$$\lim_{N,q\to\infty} (\psi_N(\beta, \boldsymbol{H}; q) - \psi'_N(\beta, \boldsymbol{H}; q)) = 0. \tag{A1.2}$$

The proof is immediate, using the inequalities

$$J'|\mathscr{H} - \mathscr{H}'| \leq (2q)^{-1} n \sum_{i,j=1}^{N} |B_{ij} - B'_{ij}| + |(2q)^{-1} - (2q')^{-1}| n \sum_{i,j=1}^{N} B'_{ij}$$

$$= \tfrac{1}{2} Nn \left(N^{-1}q^{-1} \sum_{i,j=1}^{N} |B_{ij} - B'_{ij}| + |1 - q'/q|\right) \tag{A1.3}$$

and

$$Nq|1-q'/q| \leq \sum_{i,j=1}^{N} |B_{ij}-B'_{ij}| \tag{A1.4}$$

for a direct computation of $(\psi_N^n - \psi_N'^n)$ and by passing to the limits.

Note that, if condition (A1.1) is satisfied and $\underline{\lim}\, \psi_N^n = \overline{\lim}\, \psi_N'^n = \psi$, it follows that $\lim \psi_N^n = \lim \psi_N'^n = \psi$, as used for simplicity in the proof of the theorem.

A matrix A' with the properties stated in the text can be obtained, for example, as follows.

Starting with matrix A, choose j_1 such that $q_{j_1} \geq q_i$ for all i and a set J_1, consisting of $[q_{j_1} - q]+1$ indices 'interacting' with the index j_1. Then set

$$A_{kl}^{(1)} = A_{lk}^{(1)} = \begin{cases} 0 & \text{for } k=j_1 \text{ and } l \text{ in } J_1 \\ A_{kl} & \text{otherwise.} \end{cases} \tag{A1.5}$$

With $A^{(1)}$ standing for A, $\Sigma_j A_{ij}^{(1)}$ for q_i, but keeping q the same as before, define in the same manner a matrix $A^{(2)}$. Continue this algorithm until, for some m, $[q_i^{(m)} - q]+1 \leq 0$, $i=1,\ldots,N$. Denote by A' the matrix $A^{(m)}$.

Condition (A1.1) is then fulfilled for the matrices A and A'. Indeed

$$\sum_{i,j=1}^{N} |A_{ij}-A'_{ij}| = \sum_{i,j=1}^{N} (A_{ij}-A'_{ij}) \leq 2 \sum_{\{i|q_i \geq q\}} (q_i - q) + 2N$$

$$\leq 2\sum_{i=1}^{N} |q_i - q| + 2N = 2qN\varepsilon_{N,q} + 2N. \tag{A1.6}$$

As a consequence of (A1.6) and (A1.4)

$$\lim_{q\to\infty} q'/q = 1 \tag{A1.7}$$

and also

$$q \geq \max_i q'_i. \tag{A1.8}$$

As shown by one of the referees through a bond-moving algorithm, one can prove that any matrix of form (1.2)-(1.5) is equivalent to a $|q_i - q| \leq 1$ matrix and this could be an alternative approach to the problem.

Appendix 2

Our aim here is to prove that

$$\lim_{N,q\to\infty} E_{N,q}(\alpha, 0) = 0 \tag{A2.1}$$

with $E_{N,q}(\alpha, \varepsilon)$ given by (2.10).

The eigenvalues of the matrix $I - z^{-1}K$ are

$$\lambda_i = 1 - \alpha^{-1} q^{-1} |a'_i| = 1 - z^{-1} x_i \tag{A2.2}$$

and thus

$$E_{N,q}(\alpha, 0) = \tfrac{1}{2} n\beta\, \overline{\log(1 - z^{-1}x_i)} \tag{A2.3}$$

where $\overline{y_i}$ stands for $N^{-1}\Sigma_i y_i$. As $0 \leq x_i \leq 1$, we have

$$\overline{x_i}\log(1-z^{-1}) \leq \overline{\log(1-z^{-1}x_i)} \leq 0. \tag{A2.4}$$

From the definition (A2.2) of x_i,

$$\overline{x_i^2} = N^{-1}q^{-2}\alpha^{-2}\,\mathrm{Tr}(A'^2). \tag{A2.5}$$

By construction, matrix A' has the special form (1.2). As a consequence of this and of (A1.8), the right-hand term of (A2.5) is given by

$$\alpha^{-2}q^{-2}q' \leq \alpha^{-2}(q')^{-1} \tag{A2.6}$$

so that $\lim_{N,q\to\infty}\overline{x_i^2} = 0 = \lim_{N,q\to\infty}\overline{x_i}$, which, together with (A2.4) and (A2.3), implies the result (A2.1).

References

Pearce P A 1977 *J. Phys. A: Math. Gen.* **10** 1009-22
Pearce P A and Thompson C J 1975 *Commun. Math. Phys.* **41** 191-201
—— 1978 *Commun. Math. Phys.* **58** 131-8
Thompson C J 1974 *Commun. Math. Phys.* **36** 255-62
Thompson C J and Silver H 1973 *Commun. Math. Phys.* **33** 53-60