Cluster variation method and disorder varieties of two-dimensional Ising-like models

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I show that the cluster variation method, long used as a powerful hierarchy of approximations for discrete (Ising-like) two-dimensional lattice models, yields exact results on the disorder varieties which appear when competitive interactions are put into these models. I consider, as an example, the plaquette approximation of the cluster variation method for the square lattice Ising model with nearest-neighbor, next-nearest-neighbor, and plaquette interactions, and, after rederiving known results, report simple closed-form expressions for the pair and plaquette correlation functions.

I. INTRODUCTION

The cluster variation method (CVM) is a powerful hierarchy of approximations for lattice models of equilibrium statistical mechanics which has been invented by Kikuchi[1] and more recently rewritten by An[2] and Morita.[3] It is particularly well suited to analyze complex phase diagrams of discrete classical models,[4] but in some simple cases it is also known to give exact results. Since the approximations involved amount to neglecting correlations except for a finite range, exact results are obtained whenever correlations have a particularly simple structure, as in treelike lattices[5–8] or one-dimensional strips.[9]

The purpose of the present paper is to study the behavior of the CVM in another situation in which correlations are particularly simple, namely, in the case of disorder varieties of two-dimensional Ising-like models with competitive interactions. Disorder varieties are known since the papers by Stephenson[10,11] and have subsequently been studied by many authors.[12–19] On a disorder variety (which is a suitable subspace in the whole parameter space of a model) the correlation functions factorize in a simple way, which leads to an effective dimensional reduction of the model, so one could expect that the CVM might be particularly accurate or even exact in such a case. This is indeed the case and I shall show, giving both general arguments and a detailed analysis of a particular model, that the CVM is exact on disorder varieties.

The plan of the paper is as follows: in Sec. II I shall introduce disorder varieties and briefly recall some of the results which have been obtained in the past years; Sec. III will be devoted to the definition and explanation of the CVM; in Sec. IV the exactness of the CVM on disorder varieties will be shown and finally, conclusions will be drawn in Sec. V.

II. DISORDER VARIETIES

A disorder variety is a subspace of the parameter space of a model with competitive interactions, lying in the disordered phase, where the correlations have a particularly simple form and the model can then be integrated exactly. One example of such a variety has been found by Stephenson[10] in the anisotropic antiferromagnetic Ising model on the triangular lattice. The Hamiltonian of the model can be written in the form

$$H=-\sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j, \tag{1}$$

where $\sigma_i=\pm 1$ is the spin variable at site i, the sum is over all nearest-neighbor (NN) pairs, and J_{ij} depends only on the direction of the link between sites i and j. The values of J_{ij} along the three lattice directions will be denoted by J_1, J_2, and J_3. In the antiferromagnetic model we have $J_l<0$ for $l=1,2,3$. Stephenson showed that when the condition

$$\tanh K_3+\tanh K_1\tanh K_2=0, \quad K_l=J_l/k_BT \tag{2}$$

(or one which is obtained from it by a cyclic permutation of the indices) holds, then the pair correlation along a lattice direction has a simple exponential form, as for the one-dimensional model. If σ_i and σ_j are two spin variables separated by a distance k on a linear chain of the lattice in the lth direction, their correlation $\langle\sigma_i\sigma_j\rangle$ is the kth power of the NN correlation along the same direction. In particular, assuming $J_1<J_2<J_3<0$, one has $\langle\sigma_i\sigma_j\rangle=[\tanh(K_1)]^k$ in direction 1, $\langle\sigma_i\sigma_j\rangle=[\tanh(K_2)]^k$ in direction 2 and $\langle\sigma_i\sigma_j\rangle=[\tanh(-K_3)]^k$ in direction 3. Stephenson also showed that the disorder variety separates a portion of the disordered phase in which the pair correlation has an oscillating behavior from one in which it decreases monotonically. Similar results have been obtained by the same author[11] for the union jack lattice and for certain one-dimensional lattices.

Later, Enting[12] showed that the interaction round a face (IRF) model on the square lattice [and in particular the Ising model with NN, next-nearest-neighbor (NNN), and plaquette interactions] has a disorder variety which can be mapped onto an exactly solvable crystal-growth model. Peschel and Emery[13] rederived Stephenson's results for the correlations on the disorder variety of the triangular Ising model by means of a one-dimensional kinetic model and applied this technique also to the axial NNN Ising model. Peschel and Rys[14] solved the eight vertex model on one of its disorder varieties.

Baxter[15] analyzed the disorder varieties of the IRF model on the square lattice. He showed that the eigenvector of the (diagonal to diagonal) transfer matrix corresponding to the

largest eigenvalue can be written in a simple form as the product of a sequence of two-site (NN) factors. Rujàn[16] studied the relations between different techniques and considered several models (vertex models, staggered IRF model, q-state Potts models, random bond models).

Jaekel and Maillard[17] found a local criterion which characterizes disorder varieties for any dimensionality and explains the effective dimensional reduction occurring in the model: the Boltzmann weight of an elementary cell of the lattice, summed over some (suitably chosen) spins (or whatever degrees of freedom), is independent of the remaining spins. Georges *et al.*[18] used this local criterion to calculate correlation functions on the disorder varieties of three-dimensional Ising models.

To conclude this (certainly not exhaustive) brief survey of the existing literature, we mention that recently, Meyer, Anglès d'Auriac, and Maillard[19] studied the disorder varieties of the eight vertex model in the framework of a random matrix theory approach to the transfer matrix.

III. CLUSTER VARIATION METHOD

The cluster variation method (CVM) is a hierarchy of approximation techniques for discrete classical lattice models, which has been invented by Kikuchi.[1] In its modern formulation[2,3] the CVM is based on the truncation of the cumulant expansion of the variational principle of equilibrium statistical mechanics, which says that the free energy $\mathcal{F}$ of a model defined on the lattice Λ is given by

$$\mathcal{F}=\min \mathcal{F}[\rho_\Lambda]=\min \mathrm{Tr}(\rho_\Lambda H+\rho_\Lambda \ln \rho_\Lambda), \tag{3}$$

where H is the Hamiltonian of the model, $k_B T=1$ for simplicity, and the minimization must be performed with respect to a density matrix obeying the normalization constraint $\mathrm{Tr}(\rho_\Lambda)=1$.

If the model under consideration has only short-range interactions and the maximal clusters are sufficiently large the Hamiltonian can be decomposed into a sum of cluster contributions H_α and the approximate variational free energy takes the form

$$F[\{\rho_\alpha, \alpha\in M\}]=\sum_{\alpha\in M}[\mathrm{Tr}(\rho_\alpha H_\alpha)-a_\alpha S_\alpha], \tag{4}$$

where α is a cluster of sites, $\rho_\alpha=\mathrm{Tr}_{\Lambda\setminus\alpha}\rho_\Lambda$ is the cluster density matrix ($\mathrm{Tr}_{\Lambda\setminus\alpha}$ denotes a summation over all degrees of freedom except those belonging to the cluster α), $S_\alpha=-\mathrm{Tr}(\rho_\alpha \ln \rho_\alpha)$ is the cluster entropy and the coefficients a_α can be easily obtained from the set of linear equations[2,3]

$$\sum_{\beta\subseteq\alpha\in M} a_\alpha=1, \quad \forall \beta\in M. \tag{5}$$

The cluster density matrices must satisfy the following normalization and compatibility conditions

$$\mathrm{Tr}\,\rho_\alpha=1, \ \forall \alpha\in M \quad \text{and} \quad \rho_\alpha=\mathrm{Tr}_{\beta\setminus\alpha}\rho_\beta, \ \forall \alpha\subset\beta\in M. \tag{6}$$

Notice that Eq. (4) would still be exact if the density matrix ρ_Λ of the whole lattice could be written exactly as a product of cluster density matrices in the form

$$\rho_\Lambda=\prod_{\alpha\in M}(\rho_\alpha)^{a_\alpha}. \tag{7}$$

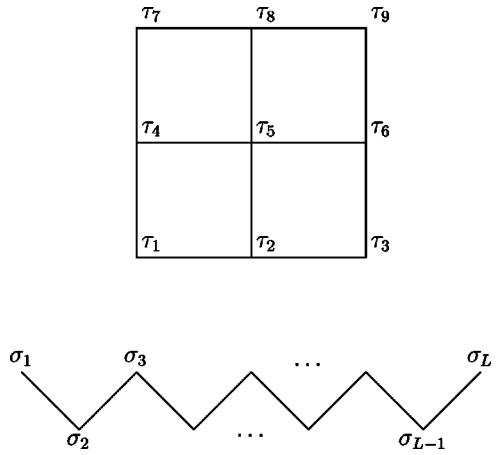

FIG. 1. The 3×3 square and the zigzag chain.

IV. EXACTNESS OF THE CLUSTER VARIATION METHOD ON DISORDER VARIETIES

There are two properties of the disorder varieties which suggest, at least for two-dimensional models, that the CVM might be exact on them. One is the one-dimensional-like character of the pair correlations. In fact, it is known that for a one-dimensional model with NN interactions, the pair approximation of the CVM (that is, the approximation in which the maximal clusters are the NN pairs), which is equivalent to the Bethe-Peierls approximation, is exact.[1,20]

The other property, still valid for two-dimensional models, is related to a result by Baxter.[15] He showed that the eigenvector (corresponding to the largest eigenvalue) of the diagonal to diagonal transfer matrix is simply the product of a sequence of two-site (NN) factors. Since the density matrix of a diagonal cluster is the square of this eigenvector also the density matrix has a product structure. As we have seen in the previous section, when the density matrix has a suitable product structure the CVM becomes exact. Therefore one can hope to find a CVM approximation which is exact on the disorder variety of a given two-dimensional model. In the square lattice case a good candidate is the plaquette approximation,[1,21] which is equivalent to the Kramers-Wannier approximation,[22] which in turn has long been known to correspond to a variational approximation in which the largest eigenvalue of the transfer matrix is searched using a restricted space of factorized vectors.[23]

In the case of the plaquette approximation for a model defined on the square lattice the condition (7), which implies the exactness of the approximation, becomes

$$\rho_\Lambda=\frac{\prod_{\mathrm{plaq}}\rho_{\mathrm{plaq}}\prod_{\mathrm{site}}\rho_{\mathrm{site}}}{\prod_{\mathrm{pair}}\rho_{\mathrm{pair}}}, \tag{8}$$

where ρ_Λ denotes the density matrix of the whole lattice and the products are to be intended over all plaquettes, pairs, and sites of the lattice. The above equation should, however, be taken with some care, since it is known that not all local thermodynamic states (i.e., density matrices) can be extended to the whole lattice.[24] Consider as an example a model of Ising spins $\sigma_i = \pm 1$ in its disordered phase, which will be studied in detail below. One can easily check on small lattices that, using a generic plaquette density matrix and the pair and site matrices derived from it by partial traces, Eq. (8) leads to a ρ_Λ which is not correctly normalized. In the case of open boundary conditions [with this choice the sites and the pairs lying at the boundary do not enter the products in Eq. (8)] the correct normalization is achieved only if $d = c^2$, where $c = \langle \sigma_i \sigma_j \rangle_{\mathrm{NN}}$ and $d = \langle \sigma_i \sigma_j \rangle_{\mathrm{NNN}}$ are the NN and NNN correlations, respectively.

When the condition $d = c^2$ holds, the procedure of extending local-density matrices to larger clusters is well defined, in the sense that by partial traces one can reobtain the local-density matrices which were used to build the larger ones. In addition, one can verify that the density matrix of any cluster admits a decomposition into a product of plaquette, pair, and site density matrices, with exponents given by the CVM rules. For instance, with reference to Fig. 1, in the case of the 3×3 square we have

$$\rho_9(\tau_1, \ldots, \tau_9) = \frac{\rho_{\mathrm{plaq}}(\tau_1, \tau_2, \tau_5, \tau_4)\rho_{\mathrm{plaq}}(\tau_2, \tau_3, \tau_6, \tau_5)\rho_{\mathrm{plaq}}(\tau_4, \tau_5, \tau_8, \tau_7)\rho_{\mathrm{plaq}}(\tau_5, \tau_6, \tau_9, \tau_8)\rho_{\mathrm{site}}(\tau_5)}{\rho_{\mathrm{pair}}(\tau_2, \tau_5)\rho_{\mathrm{pair}}(\tau_5, \tau_8)\rho_{\mathrm{pair}}(\tau_4, \tau_5)\rho_{\mathrm{pair}}(\tau_5, \tau_6)}, \tag{9}$$

while for the zigzag chain

$$\rho_{\mathrm{chain}}(\sigma_1, \sigma_2, \ldots, \sigma_L) = \frac{\rho_{\mathrm{pair}}(\sigma_1, \sigma_2)\rho_{\mathrm{pair}}(\sigma_2, \sigma_3) \ldots \rho_{\mathrm{pair}}(\sigma_{L-1}, \sigma_L)}{\rho_{\mathrm{site}}(\sigma_2)\rho_{\mathrm{site}}(\sigma_3) \ldots \rho_{\mathrm{site}}(\sigma_{L-1})}. \tag{10}$$

As a consequence, also the pair-correlation function has a very simple product form, that is (labeling the spin variables by the site coordinates)

$$g(x,y) = \langle \sigma(x_0, y_0)\sigma(x_0 + x, y_0 + y) \rangle = c^{|x| + |y|}. \tag{11}$$

The result (10) is equivalent to the result by Baxter[15] that, on disorder varieties, the eigenvector of the diagonal to diagonal transfer matrix, corresponding to the largest eigenvalue, can be written as a product of NN pair terms. ρ_{chain} is just the square of this eigenvector, and the site factors which appear in the denominator can be easily associated, in a symmetric way, to the adjacent pairs. This shows (although this is not a rigorous proof) that when the plaquette approximation is exact for a model of Ising spins on the square lattice, then the model is at a point of the disorder variety in its parameter space.

Let us finally study in detail the square lattice Ising model with NN, NNN, and plaquette interactions. The Hamiltonian of the model can be written in the form

$$H = -J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_2 \sum_{\langle\langle ij \rangle\rangle} \sigma_i \sigma_j - J_4 \sum_{\substack{j \\ k \square \, i \\ l}} \sigma_i \sigma_j \sigma_k \sigma_l, \tag{12}$$

where J_1, J_2, and J_4 are the NN, NNN, and plaquette couplings, respectively. This is a special case of the models studied in Refs. 12, 15, 16, and 19. We shall first use the plaquette approximation of the CVM. Notice that this approximation has already been applied to the same model in Refs. 21 and 25–27. In particular, Sanchez[21] reported closed-form expressions for the equilibrium density matrices and the momentum space pair-correlation function in the disordered phase. Morán-López, Aguilera-Granja, and Sanchez[25] observed qualitatively the existence of a disorder locus in the phase diagram. Cirillo *et al.*[27] calculated again the momentum space pair-correlation function, and on this basis they determined the location of the disorder line. Their pair-correlation function coincides with that by Sanchez except for a misprint,[28] and they obtained a disorder line which is only very close to the exact one, instead of coincident as it should be on the basis of the results of the present paper, because of an additional approximation.

As a first step one can, at least at the numerical level, verify that the approximation is exact on the disorder variety using only the CVM. A simple way is to consider a hierarchy of approximations like the so-called C series,[29] in which the maximal cluster is a rectangle made of $2 \times L$ sites, with $L \geqslant 2$ (the plaquette approximation is the first element of the C series). It is found, with extremely high precision, that a sequence of approximations in this series gives identical results on the disorder variety of the model. Inspection of the pair correlations shows that Eq. (11) is also satisfied.

On the other hand, using published results[21] it requires only a long but straightforward calculation to check that on the (known[12,14,19]) disorder variety of the model one obtains the exact free energy. Looking at the pair correlations one also sees that the condition $d = c^2$ [see Eq. (11)] is satisfied on the variety of equation

$$\cosh(2J_1) = \frac{\exp(2J_4)\cosh(4J_2) + \exp(-2J_2)}{\exp(2J_2) + \exp(2J_4)}, \tag{13}$$

which is precisely the disorder variety of the model.[12,19] The free energy per site can be written as

$$f = -\ln[\exp(-J_4) + \exp(J_4 - 2J_2)], \tag{14}$$

and again coincides with the exact one, while the NN correlation is

$$c=\frac{\exp(-4J_2)-\cosh(2J_1)}{\sinh(2J_1)}, \tag{15}$$

the NNN correlation $d=c^2$, and the plaquette correlation

$$q=\langle\sigma_i\sigma_j\sigma_k\sigma_l\rangle=\frac{\exp(4J_4)[1-\exp(8J_2)]+4\exp(2J_2)[\exp(2J_4)-\exp(2J_2)]}{\exp(4J_4)[1-\exp(8J_2)]+4\exp(2J_2)[\exp(2J_4)+\exp(2J_2)]}. \tag{16}$$

Finally, since all the pair correlations are given simply by Eq. (11) we can easily calculate the momentum space correlation function, or structure factor. We first rewrite Eq. (11) as $g(x,y)=\exp[-(|x|+|y|)/\xi]$, where $\xi=-(\ln c)^{-1}$. After a Fourier transform one finds $S(p_x,p_y)=S_1(p_x)S_1(p_y)$, where

$$S_1(p)=\frac{\sinh(1/\xi)}{\cosh(1/\xi)-\cos p}. \tag{17}$$

It can be verified that the structure factors calculated by Sanchez[21] and (except for the misprint) Cirillo *et al.*[27] reduce to the above expression on the disorder line.

V. CONCLUSIONS

I have shown that the CVM gives exact results on the disorder varieties of two-dimensional Ising-like models. In particular, I have considered the Ising model with NN, NNN, and plaquette interactions on the square lattice, in the plaquette approximation of the CVM. In the disordered phase of the model, imposing the simple condition that the NNN pair correlation equals the square of the NN pair correlation, the CVM plaquette approximation becomes exact and it is shown that this condition holds on the disorder variety, where the model can be solved in closed form. It is important to notice that, using the CVM, one can obtain any correlation function, due to the fact that the procedure of extending the local thermodynamic state is well defined just on the disorder variety. Similar results can be obtained on the triangular lattice as well as other two-dimensional lattices.

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