Constraints on high-temperature series expansions for spin correlations in the square Ising model

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High-temperature series expansions have been derived for pair correlations in the square Ising model with nearest-neighbor and diagonal interactions. Enting has pointed out that constraints on the series expansions can be obtained from exact results on the disorder line of the model. The constraints are imposed on the pair correlation series and turn out to be satisfied by the published series coefficients. The coefficients thus pass a rather severe test. In addition, the constraints allow the prediction of a few extra coefficients.

I. CRYSTAL-GROWTH MODEL AND ISING-MODEL DISORDER LINE

The aim of this report is twofold. Firstly, a partial check is provided of the coefficients of high-temperature series for Ising-spin correlations published by Indekeu, Stella, and Rogiers.[1] Secondly, a further example is given of the derivation by Enting[2] of constraints on series expansions from the knowledge of an exact solution of the model for special sets of interaction parameters commonly referred to as disorder points.[3]

In the following use will be made of the relationship between Ising models at their disorder points and crystal-growth models, as demonstrated by Enting.[4] The Ising model that we consider is defined on the square lattice (in two dimensions) by the following reduced Hamiltonian:

$$-\beta H(\{\sigma\}) = K\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'} + L\sum_{\langle\langle \mathbf{r}\mathbf{r}'\rangle\rangle}\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'} , \tag{1}$$

where $\beta = 1/k_B T$. The Ising spins $\sigma_{\mathbf{r}} (= \pm 1)$ interact via (reduced) nearest-neighbor coupling K and next-nearest-neighbor or diagonal coupling L.

The probability distribution for spin configurations $\{\sigma\}$ is given by

$$P(\{\sigma\}) = \exp[-\beta H(\{\sigma\})]/Z , \tag{2}$$

where Z is the canonical partition function.

The pertinent crystal-growth model on the square lattice is defined by the following probability distribution for configurations of occupation variables $\{x\}$:

$$P(\{x\}) = \prod_{\mathbf{r}} P_{\mathbf{r}}(\{x\}) , \tag{3}$$

with

$$P_{\mathbf{r}}(\{x\}) = P_c(x_{\mathbf{r}} \mid x_{\mathbf{r}-\mathbf{a}-\mathbf{b}}, x_{\mathbf{r}-\mathbf{b}}, x_{\mathbf{r}-\mathbf{a}}) , \tag{4}$$

where $\mathbf{a}$ and $\mathbf{b}$ are unit vectors along the principal lattice axes, and P_c is a conditional probability. As a consequence, the occupation of site $\mathbf{r}$ is made to depend only on the occupations of neighboring "predecessor" sites.[4] After making the correspondence between occupation variables x and Ising spin variables σ through $x = (1+\sigma)/2$, the requirement that P_c be a conditional probability is expressed as

$$\sum_{\sigma_{\mathbf{r}}} P_c(\sigma_{\mathbf{r}} \mid \sigma_{\mathbf{r}-\mathbf{a}-\mathbf{b}}, \sigma_{\mathbf{r}-\mathbf{b}}, \sigma_{\mathbf{r}-\mathbf{a}}) = 1 . \tag{5}$$

Assuming furthermore spin-reversal symmetry (i.e., atom-vacancy symmetry) P_c must take the form

$$P_c(\sigma_4 \mid \sigma_1, \sigma_2, \sigma_3) = \tfrac{1}{2} + \sigma_4 (A\sigma_2 + A'\sigma_3 + B\sigma_1 + C\sigma_1\sigma_2\sigma_3) , \tag{6}$$

where the labeling is such that σ_2 and σ_3 are nearest neighbors of σ_4, and σ_1 is diagonally across from σ_4, in an elementary square on the lattice.

The solubility of the crystal-growth model relies on the property (4) which allows the derivation of simple closed sets of equations for the spin correlations. The Ising probability distribution (2) can be factorized in conditional probabilities (4) provided a specific relationship is imposed between the couplings K and L.

One can write

$$P_c(\sigma_4 \mid \sigma_1, \sigma_2, \sigma_3) = \exp\{-\beta[E(\sigma_1, \sigma_2, \sigma_3, \sigma_4) - \Delta]\} , \tag{7}$$

where, most generally and respecting spin-reversal symmetry,

$$-\beta E = K_a\sigma_1\sigma_2 + K_a'\sigma_3\sigma_4 + K_b\sigma_1\sigma_3 + K_b'\sigma_2\sigma_4 + L_1\sigma_1\sigma_4 + L_2\sigma_2\sigma_3 + F\sigma_1\sigma_2\sigma_3\sigma_4 . \tag{8}$$

The couplings $K_a, \ldots, F$ can be expressed in terms of

$$P_1 \equiv P_c(+ \mid +++) ,$$
$$P_2 \equiv P_c(+ \mid ++-) ,$$
$$P_3 \equiv P_c(+ \mid +-+) ,$$
$$P_4 \equiv P_c(+ \mid -++) ,$$

using (5) and (7).

The product over all sites $\mathbf{r}$ of the exponential in (7) gives an expression of the form (2). In order to obtain complete correspondence with the Ising model defined in (1), one must have

$$K_a + K_a' = K_b + K_b' = K , \tag{9}$$

$$L_1 = L_2 , \tag{10}$$

$$F = 0 , \tag{11}$$

$$-\beta\Delta = (\ln Z)/N , \tag{12}$$

assuming N lattice sites.

The requirements (9)–(11) imply, in the crystal-growth model,

$$P_2 = P_3 \quad (\text{or } A = A') \ , \tag{13}$$

$$P_2 P_3 = (1 - P_1) P_4 \ , \tag{14}$$

$$P_1 (1 - P_2)(1 - P_3)(1 - P_4) = (1 - P_1) P_2 P_3 P_4 \ , \tag{15}$$

respectively. It also follows that

$$K_a = K_b, \ K_a' = K_b' \ . \tag{16}$$

Requirement (12), which expresses that Δ is the free energy per site, is in general incompatible with (7), because in (7) Δ must take care of the proper *normalization* of the conditional probability P_c. However, in a special case both requirements can be met simultaneously. Imposing the normalization (5) one finds the desired special Ising model with *constraints* on the interactions:

$$\exp(4K_a) = \frac{\cosh(2K_a' - L)}{\cosh(2K_a' + L)} \ , \tag{17}$$

$$[\exp(-4L) - 1](\cosh L)^2 = (\sinh 2K_a')^2 \ . \tag{18}$$

Furthermore,

$$-\beta\Delta = \ln[1 + \exp(-2L)] \ . \tag{19}$$

These relations, together with (9), define the disorder line of the Ising model and the corresponding (trivial) free energy. The disorder line lies entirely in the subspace of antiferromagnetic diagonal coupling ($L < 0$), and in the paramagnetic phase. This line is shown, e.g., in Fig. 3(c) of Ref. 4 and Fig. 2 of Ref. 5. For small couplings it is approximately given by

$$-L \simeq K^2 \ . \tag{20}$$

On the disorder line the pair correlations have been derived by Enting.[6] His result for our case of full square lattice symmetry can be written in the form

$$\langle \sigma_0 \sigma_{m\mathbf{a}+n\mathbf{b}} \rangle = (\tanh K_{1D})^{|m|+|n|} \ , \tag{21}$$

where $K_{1D} \equiv K_a' - K_a$. The notation K_{1D} makes reference to the Ising model in one dimension where a similar decay holds for the pair correlation function. Result (21) means that on the disorder line the competition between the nearest-neighbor interaction and the antiferromagnetic diagonal interaction is such that correlations effectively propagate only along a path that consists of the smallest number of nearest-neighbor steps connecting the sites.

II. CONSTRAINTS ON SERIES EXPANSIONS FOR SPIN CORRELATIONS

In 1985, Indekeu, Stella, and Rogiers constructed static and dynamic real-space renormalization-group (RG) transformations through series expansions for correlation functions.[1] They applied the RG approach to the square Ising model with nearest-neighbor and diagonal interactions. For implementing the static scheme they derived high-temperature series to ninth order (in both interactions) for seven pair correlations. These series expansions of $\langle \sigma_0 \sigma_{\mathbf{r}} \rangle$ are denoted by

$$G_9(\mathbf{v}, \mathbf{r}) = \sum_{i+j=1}^{9} a_{ij}(\mathbf{r}) v^i w^j \ , \tag{22}$$

where $\mathbf{v} = (v, w)$, $v = \tanh K$, and $w = \tanh L$. The coefficients a_{ij} are tabulated in Tables XXXIII through XXXIX in Ref. 1. The computations were done for $\mathbf{r} = \mathbf{a}$, $2\mathbf{a}$, $3\mathbf{a}$, $4\mathbf{a}$, $6\mathbf{a}$, $\mathbf{a}+\mathbf{b}$, and $2\mathbf{a}+2\mathbf{b}$.

It is now straightforward to obtain constraints on the series expansions. From (17) and (18) one derives the following expansions of K_a and L in powers of $y \equiv K_a'$:

$$L = -y^2 + \tfrac{2}{3} y^4 + \tfrac{13}{45} y^6 - \tfrac{988}{315} y^8 + \tfrac{108868}{14175} y^{10} + \cdots \ , \tag{23}$$

$$K_a = y^3 - 2y^5 + \tfrac{12}{5} y^7 + \tfrac{206}{189} y^9 - \tfrac{67093}{4725} y^{11} + \cdots \ . \tag{24}$$

Expansions for $K = K_a + K_a'$ and $K_{1D} = K_a' - K_a$ follow immediately. The constraints now obtain by requiring that (21) and (22) have identical expansions in the variable y. This requirement allows a partial check of the coefficients a_{ij}. Note that K and $v = \tanh K$ are of first order in y, whereas L and $w = \tanh L$ are of second order in y. As a consequence, the check can be performed up to (and including) ninth order in v but only fourth order in w. Interestingly, one can go a little further when making additional use of the coefficients of v^{10} and v^{11} derived by Fisher and Burford.[7] This allows to make the check complete up to (and including) tenth order in v and fifth order in w, and to make a *prediction* for the coefficient of $v^9 w$. This coefficient was not previously derived[1] but can be expressed in terms of the coefficients of v^{11}, $v^7 w^2$, $v^5 w^3$, $v^3 w^4$, and $v w^5$ through a constraint.

For calculational purposes the following results are useful:

$$v = \tanh K = y + \tfrac{2}{3} y^3 - \tfrac{43}{15} y^5 + \tfrac{1264}{315} y^7 + \tfrac{5672}{2835} y^9 - \tfrac{3848126}{155925} y^{11} + \cdots \ , \tag{25}$$

$$w = \tanh L = -y^2 + \tfrac{2}{3} y^4 + \tfrac{28}{45} y^6 - \tfrac{1198}{315} y^8 + \tfrac{109183}{14175} y^{10} + \cdots \ , \tag{26}$$

$$\tanh K_{1D} = y - \tfrac{4}{3} y^3 + \tfrac{47}{15} y^5 - \tfrac{1928}{315} y^7 + \tfrac{24692}{2835} y^9 - \tfrac{915548}{155925} y^{11} + \cdots \ . \tag{27}$$

The result of the check is that the coefficients satisfy the constraints, as they should. This does not prove that the coefficients are correct but provides a good reason for believing it. The check furthermore predicts two new coefficients: for $\mathbf{r} = \mathbf{a}$,

$$a_{9,1} = 680 \ , \tag{28}$$

and for $\mathbf{r} = 3\mathbf{a}$,

$$a_{9,1} = 2140 \ . \tag{29}$$

(The coefficient $a_{9,1}$ is trivially zero for the other five pair correlations under consideration.)

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