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# Consistent Relations in the Method of Reducibility in the Cluster Variation Method

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A redundancy is noted in the set of Lagrange multipliers—effective fields and effective interactions—used in the expressions of the reduced density matrices given by Morita[4] in some problems with less symmetry.[6] The expressions of the reduced density matrices without this redundancy are given. An argument showing that a certain expression of the free energy in terms of the Lagrange multipliers is stationary with respect to the variations of these is presented.

**KEY WORDS:** Cluster variation method; effective field; effective interaction; reduced density matrices; reducibility condition; variational principle.

## 1. INTRODUCTION

The cluster variation method[1] presents an approximate method which gives the properties of the Ising model and the Heisenberg model. In that method, an approximate free energy of the system is expressed in terms of the reduced density matrices, and the reduced density matrices are determined by the minimum of that expression of the free energy, where the variations are taken with the restriction that the reduced density matrices should satisfy the reducibility relations between them.[2,3]

In the general condition, the variation was taken by the author,[4] introducing a Lagrange multiplier for each of the restrictions. In the result of the variational calculation, the reduced density matrices are expressed in terms of the Lagrange multipliers, each of which is interpreted as an effective field or an effective interaction, and these are determined by the reducibility of the reduced density matrices.

This method of the reducibility manifested to be a convenient starting point in getting the result of an approximation in the cluster variation

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method, for a simple ferromagnet or antiferromagnet.[5] However, in applying it to the Ising model with an antiferromagnetic interaction on the fcc lattice, Fujiki[6] found that there are cases where the number of the consistent relations in the reducibility condition is less than the number of Lagrange multipliers or the effective fields and effective interactions. In those cases, the number of the linearly independent expressions of the linear combinations of a set of Lagrange multipliers expressing the reduced density matrices is less than the total number of the Lagrange multipliers in the set. That is, the reduced density matrices are determined by the linearly independent expressions, before all the Lagrange multipliers are determined. Although we get the correct result of the cluster variation method without determining undetermined Lagrange multipliers, it is not convenient to have redundant Lagrange multipliers. In the present paper, an improved recipe is given of the method of reducibility in the cluster variation method.

In previous papers,[3,4] it is stated that the Lagrange multipliers can be determined by the stationariness with respect to their variations of a certain expression of the free energy. An argument showing this fact was given in a footnote of Ref. 3 only for the most simple case. An argument showing this fact for the present case is given in Section 5. The obtained results are summarized in Section 6. An example is given in Section 7.

Notations follow Ref. 4, if not stated otherwise. For example, $n \subseteq m$ and $n \subset m$ are used to indicate that $n$ is a subcluster and a proper subcluster of $m$, respectively.

## 2. VARIATIONAL FUNCTION

An approximation in the cluster variation method is characterized by a set of preserved clusters $M_i$ of sites. We consider the clusters $M_i$ and the common parts of two, three, ... of $M_i$'s, that is, $M_i, M_i \cap M_j, M_i \cap M_j \cap M_k, \ldots$. We denote the set of all these clusters, excluding the cluster having no sites, by $U$. We assume that the Hamiltonian of the system $H$ is expressed as a sum of contributions $h^\dagger(n)$ of the clusters $n$ belonging to $U$:

$$H = \sum_n^\dagger h^\dagger(n) \tag{2.1}$$

where $\dagger$ above the summation sign denotes the restriction $n \in U$. In the method, the approximate free energy is expressed in terms of the reduced density matrices of the clusters belonging to $U$.

The approximate free energy is given by

$$F = \sum_n^\dagger \mathrm{tr}_n \rho(n) h^\dagger(n) + \sum_n^\dagger \gamma^\dagger(n) \tag{2.2}$$

where $\gamma^{\dagger}(n)$ is defined by

$$\Gamma(m) = kT \operatorname{tr}_m \rho(m) \ln \rho(m) \tag{2.3}$$

and

$$\Gamma(m) = \sum_{\substack{n \\ (n \subseteq m)}}^{\dagger} \gamma^{\dagger}(n) \tag{2.4}$$

Here $k$ is the Boltzmann constant, $T$ is the temperature, and $\rho(m)$ is the reduced density matrix for the cluster $m$. If $m$ has no proper subcluster included in $U$, $\gamma^{\dagger}(m) = \Gamma(m)$ and if otherwise (2.4) is written as $\gamma^{\dagger}(m) = \Gamma(m) - \sum_{n(n \subset m)}^{\dagger} \gamma^{\dagger}(n)$, which is used to get $\gamma^{\dagger}(m)$, recursively.

In the cluster variation method, the reduced density matrices $\rho(m)$ are so determined that $F$ defined by (2.2)–(2.4) is stationary with respect to the variations of $\rho(m)$, where the reducibility relations and the normalization conditions are required. The reducibility relations required are

$$\rho(m') = \operatorname{tr}_{m \setminus m'} \rho(m) \tag{2.5}$$

between those clusters $m$ and $m'$ that $m \in U$, $m' \in U$, $m' \subset m$ and there is no $m''$ such that $m'' \in U$ and $m' \subset m'' \subset m$. The normalization conditions are

$$\operatorname{tr}_m \rho(m) = 1 \tag{2.6}$$

for $m$ belonging to $U$.

## 3. INDEPENDENT SET OF REDUCIBILITY CONDITIONS

We introduce a linearly independent set of operators for a cluster $m$ belonging to $U$, in such a way that the set involves the set for every cluster $n$ which is a subcluster of $m$ and belongs to $U$. The set involves the operator 1. An operator in the set is denoted by $Q_{\nu}^{\dagger}(n)$ if it is involved in the set for the cluster $n$ but is not equal to unity nor involved in the set for any of its subclusters included in $U$; $\nu$ is used to distinguish different ones satisfying this condition.

In Ref. 4, a Lagrange multiplier $\lambda(m - m'; m')$ is introduced to secure the reducibility (2.5) of the reduced density matrix for the cluster $m$ to that for $m'$ if $m \in U$, $m' \in U$, $m' \subset m$, and there is no $m''$ such that $m'' \in U$ and $m' \subset m'' \subset m$.

If we use the complete set of linearly independent operators $Q_{\nu}^{\dagger}(n)$, (2.5) is equivalent to the set of conditions:

$$\operatorname{tr}_{m'} Q_{\nu}^{\dagger}(n) \rho(m') = \operatorname{tr}_m Q_{\nu}^{\dagger}(n) \rho(m) \tag{3.1}$$

for all the subclusters $n$ of $m$, satisfying $n \in U$ and $n \subseteq m'$, if the normalizations of $\rho(m')$ and $\rho(m)$ are secured.

In a study applying the method of reducibility to an antiferromagnetic Ising model on the fcc lattice, Fujiki[6] found a redundancy in the Lagrange multipliers. It occurs for the Lagrange multipliers for (3.1) when there is another cluster $m''$ such that $m'' \in U$ and $n \subset m'' \subset m$. Then we have a reducibility of $\rho(m')$ to $\rho(n)$, $\rho(m'')$ to $\rho(n)$ and also $\rho(m)$ to $\rho(m'')$, so that

$$\mathrm{tr}_n Q_\nu^\dagger(n)\rho(n) = \mathrm{tr}_{m'} Q_\nu^\dagger(n)\rho(m') \tag{3.2}$$

$$\mathrm{tr}_n Q_\nu^\dagger(n)\rho(n) = \mathrm{tr}_{m''} Q_\nu^\dagger(n)\rho(m'') \tag{3.3}$$

$$\mathrm{tr}_{m''} Q_\nu^\dagger(n)\rho(m'') = \mathrm{tr}_m Q_\nu^\dagger(n)\rho(m) \tag{3.4}$$

When we include (3.2) and (3.3) in the set of subsidiary conditions, we have only to include one of (3.1) and (3.4), and then the other is automatically satisfied. Hence we can discard it from the set of subsidiary conditions. An alternative way is to use

$$\mathrm{tr}_n Q_\nu^\dagger(n)\rho(n) = \mathrm{tr}_m Q_\nu^\dagger(n)\rho(m) \tag{3.5}$$

along with (3.2) and (3.3), since (3.1) and (3.4) are automatically satisfied if (3.2), (3.3), and (3.5) are satisfied.

In summary, we have only to introduce Lagrange multipliers $\lambda_\nu^\dagger(m-n,n)$ for the consistency conditions (3.5) for all $n$ and all $m$ satisfying $n \in U$, $m \in U$ and $n \subset m$. In addition to these, we have the Lagrange multipliers $f^\dagger(m)$ to secure the normalization conditions (2.6).

## 4. VARIATIONAL CALCULATION

We introduce the Lagrange multipliers $\lambda_\nu^\dagger(m-n,n)$ and $f^\dagger(m)$ for the subsidiary conditions (3.5) and (2.6), respectively, and rewrite the variational function given by (2.2) as follows:

$$\mathscr{F} = \sum_n{}^\dagger \mathrm{tr}_n \rho_t(n)\left[h^\dagger(n) + \lambda^\dagger(n) - f^\dagger(n)\right] + \sum_n{}^\dagger\left[\gamma^\dagger(n) + f^\dagger(n)\right], \tag{4.1}$$

where $\gamma^\dagger(n)$ here is defined by (2.3) and (2.4) if $\rho(m)$ in (2.3) are replaced by $\rho_t(m)$, and $\lambda^\dagger(n)$ are defined by

$$\lambda^\dagger(n) = -\sum_{\substack{n' \\ (n' \subset n)}}{}^\dagger \sum_\nu \lambda_\nu^\dagger(n-n',n') Q_\nu^\dagger(n') + \sum_{\substack{m \\ (m \supset n)}}{}^\dagger \sum_\nu \lambda_\nu^\dagger(m-n,n) Q_\nu^\dagger(n) \tag{4.2}$$

Here the variations are to be taken with respect to $\rho_t(m)$.

We shall rewrite (4.1) by adding $\lambda_\nu^\dagger(m-n,n)$ and $f^\dagger(n)$ some adequate

constants as follows:

$$\mathscr{F} = \sum_n^{\dagger} \mathrm{tr}_n \rho_t(n)\left[ h^{\dagger}(n) + \lambda^{\dagger}(n) + kT \ln g^{\dagger}(n) - f^{\dagger}(n) \right] + \sum_n^{\dagger} \left[ \gamma_3(n) + f^{\dagger}(n) \right] \tag{4.3}$$

where $\gamma_3(n)$ are defined by

$$\Gamma_3(m) = kT \,\mathrm{tr}_m \rho_t(m)\left[ \ln \rho_t(m) - \ln \rho(m) - 1 \right] + kT \tag{4.4}$$

$$\Gamma_3(m) = \sum_{\substack{n \\ (n \subseteq m)}}^{\dagger} \gamma_3(n) \tag{4.5}$$

and $\ln g^{\dagger}(n)$ are defined by

$$\ln \rho(m) = \sum_{\substack{n \\ (n \subseteq m)}}^{\dagger} \ln g^{\dagger}(n) \tag{4.6}$$

Here $\rho(m)$ are the functions to be determined as $\rho_t(m)$ which make $\mathscr{F}$ stationary.

The result of the variation is

$$\rho(m) = \exp\{ \beta\left[ F(m) - H(m) - \Lambda(m) \right] \} \tag{4.7}$$

where

$$F(m) = \sum_{\substack{n \\ (n \subseteq m)}}^{\dagger} f^{\dagger}(n) \tag{4.8}$$

$$\Lambda(m) = \sum_{\substack{n \\ (n \subseteq m)}}^{\dagger} \sum_{\substack{m' \\ (m' \supset n) \\ (m' \not\subseteq m)}}^{\dagger} \sum_{\nu} \lambda_{\nu}^{\dagger}(m' - n, n) Q_{\nu}^{\dagger}(n) \tag{4.9}$$

(4.9) is obtained by using (4.2) in $\Lambda(m) = \sum_{n \subseteq m}^{\dagger} \lambda^{\dagger}(n)$. In order to determine the Lagrange multipliers, we use the normalization (2.6) for $F(m)$ and the relation (3.5) for $\lambda_{\nu}^{\dagger}(m - n, n)$. We then use (4.8) to get $f^{\dagger}(n)$ and obtain the free energy of the system $F$ by

$$F = \sum_n^{\dagger} f^{\dagger}(n) \tag{4.10}$$

In determining $\lambda_{\nu}^{\dagger}(m - n, n)$, we may use the condition of the reducibility (2.5). The set of (3.5) gives all that are required to secure (2.5). The argument in the preceding section shows that the set of (2.5) may have redundant equations which are automatically satisfied when the others are satisfied.

## 5. STATIONARINESS WITH RESPECT TO THE VARIATIONS OF LAGRANGE MULTIPLIERS

The variational free energy (4.3) is a function of $\rho_t(m)$, $\lambda_\nu^\dagger(m-n,n)$ and $f^\dagger(n)$. The conditions determining these are stationariness conditions:

$$\frac{\delta \mathscr{F}}{\delta \rho_t(m)} = 0 \tag{5.1}$$

with the subsidiary conditions (3.5) and (2.6). The latter are written as

$$\frac{\partial\{\mathscr{F} \text{ given by (4.3)}\}}{\partial \lambda_\nu^\dagger(m-n,n)} = 0 \tag{5.2}$$

$$\frac{\partial\{\mathscr{F} \text{ given by (4.3)}\}}{\partial f^\dagger(n)} = 0 \tag{5.3}$$

We shall obtain $\rho_t(m)$ and $f^\dagger(m)$ by conditions (5.1) and (5.3). Then the obtained $\rho_t(m)$ and $f^\dagger(m)$ are functions of $\lambda_\nu^\dagger(m-n,n)$. We shall substitute them into (4.3) in place of $\rho_t(m)$ and $f^\dagger(m)$. The obtained $\mathscr{F}$ is a function of $\lambda_\nu^\dagger(m-n,n)$ partly explicitly and partly implicitly through $\rho_t(m)$ and $f^\dagger(m)$. We shall refer this as to $\mathscr{F}_B$. Then

$$\begin{aligned}\frac{\partial \mathscr{F}_B}{\partial \lambda_\nu(m-n,n)} = \sum_{\substack{m' \\ (m' \supseteq n) \\ (m' \not\subseteq m)}} \Bigg\{ & \mathrm{tr}_{m'} \left[ \frac{\delta \mathscr{F}_B}{\delta \rho_t(m')} \right]_{\lambda_\nu^\dagger, f^\dagger} \frac{\partial \rho_t(m')}{\partial \lambda^\dagger{}_\nu(m-n,n)} \\ & + \left[ \frac{\partial \mathscr{F}_B}{\partial f^\dagger(m')} \right]_{\rho_t, \lambda_\nu^\dagger} \frac{\partial f^\dagger(m')}{\partial \lambda_\nu^\dagger(m-n,n)} \Bigg\} \\ & + \left[ \frac{\partial \mathscr{F}_B}{\partial \lambda_\nu^\dagger(m-n,n)} \right]_{\rho_t, f^\dagger}\end{aligned} \tag{5.4}$$

where the variations of $\mathscr{F}_B$ on the right-hand side are taken with fixed values of $\rho_t(m)$, $\lambda_\nu^\dagger(m-n,n)$ and $f^\dagger(n)$ except the one of which the variation is taken. Since the variations of $\mathscr{F}_B$ in the summand on the right-hand side in (5.4) are zero, condition (5.2), that is zero of the last term of the right-hand side, is equivalent to

$$\frac{\partial \mathscr{F}_B}{\partial \lambda_\nu^\dagger(m-n,n)} = 0 \tag{5.5}$$

Condition (5.1) gives (4.7) for $\rho(m)$, and (5.3) is equivalent to (2.6),

which determines $F(m)$ as follows:

$$\exp\left[-\beta F(m)\right] = \mathrm{tr}_m \exp\left\{-\beta\left[H(m) + \Lambda(m)\right]\right\} \tag{5.6}$$

We substitute (4.7) and (5.6) into (4.3) and obtain $\mathscr{F}_B$, that is equal to

$$\mathscr{F}_B = \sum_n^{\dagger} f^{\dagger}(n) \tag{5.7}$$

The above argument shows that if $f^{\dagger}(n)$ are calculated by (4.8) and (5.6), $\lambda_\nu^{\dagger}(m-n,n)$ must be determined by the stationariness condition (5.5) of $\mathscr{F}_B$ given by (5.7). The resulting value of $\mathscr{F}_B$ must be equal to the free energy given by (4.10).

## 6. SUMMARY

In a certain approximation of the cluster variation method, we choose a set of preserved clusters $M_i$ and construct the set $U$ of their common parts. The Hamiltonian is assumed to be given by the sum of contributions $h^{\dagger}(n)$ of clusters $n$ belonging to the set $U$, as (2.1). For each cluster $m$ belonging to $U$, a set of operators $Q_\nu^{\dagger}(m)$ is introduced such that the set of $Q_\nu^{\dagger}(m)$ along with unity and the sets $Q_\nu^{\dagger}(n)$ for all proper subclusters $n$ of $m$, belonging to $U$, constitutes a complete set of operators for the cluster $m$.

When $n$ and $m$ belong to $U$ and $n$ is a proper subcluster of $m$, an effective field or an effective interaction $\lambda_\nu^{\dagger}(m-n,n)Q_\nu^{\dagger}(n)$ is introduced to secure the consistency of the average for each of $Q_\nu^{\dagger}(n)$. The reduced density matrices $\rho(m)$ for $m$ belonging to $U$ are then given by (4.7) with (4.9). (4.9) states that the effective fields and effective interactions in $\rho(m)$ are to subclusters $n$ of $m$, belonging to $U$, from such clusters $m'$, that $m'$ belongs to $U$, $n$ is a subcluster of $m'$ and $m'$ is not a subcluster of $m$. $F(m)$ are given in terms of the set of $\lambda_\nu^{\dagger}(m-n,n)$ by the normalization condition, that is, (2.6) or (5.6). In the method of reducibility, the effective fields and effective interactions $\lambda_\nu^{\dagger}(m-n,n)$ are determined by the consistency relations (3.5). Then $F(m)$ are calculated by (5.6) and the free energy of the system is given by (4.10) and (4.8). In the method using the stationariness condition, from the expression of $F(m)$ in terms of the set of $\lambda_\nu^{\dagger}(m-n,n)$, we calculate $\mathscr{F}_B$ by (5.7) and (4.8). By the condition of stationariness (5.5) of this expression with respect to the variations of $\lambda_\nu^{\dagger}(m-n,n)$, we can determine these. The stationary value of $\mathscr{F}_B$ gives the free energy of the system.

## 7. EXAMPLE

As an example, we consider the Heisenberg model on the rectangular lattice in the rectangle approximation, where all the basic rectangles are

preserved clusters. The directions along the edges of the rectangles are called the $x$ and $y$ directions. The Hamiltonian is

$$H = -\sum_i hs_{iz} - \sum_{\substack{i>j \\ (i,j\,:\,n\cdot n)}} J_{ij} s_i \cdot s_j \tag{7.1}$$

where $h$ is the external field and $J_{ij}$ is $J_x$ or $J_y$ according to whether $i$ and $j$ are nearest neighbors in the direction parallel to the $x$ or $y$ direction. As the set of common parts of the basic rectangles, $U$ is the set of sites, nearest neighbor pairs of sites, and basic rectangles. We assume that the system is in the ferromagnetic or paramagnetic state and the magnetization is in the $z$ direction.

The reduced density matrix $\rho(m)$ for each $m$ which is an element of $U$ is expressed in the form of (4.7). When $m$ is a site, $\rho(m)$ is expressed as $\rho^{(1)}(s)$ as a function of the spin variable $s$ for the site. The set $\{Q_\nu(m)\}$ for the site is $\{s_z, s_x, s_y\}$, and $H(m) = -hs_z$. The sum (4.9) is obtained as follows: When $m$ is a site, $n$ satisfying $n \subseteq m$ and $n \in U$ is only $m$ itself, and we have only terms of $Q_\nu^\dagger(n) = s_z$ in the ferromagnetic or paramagnetic state. The $\lambda_\nu^\dagger(m' - n, n)$ for $m'$, which is a pair of the site being considered and one of its two nearest neighbors in the $x$ direction ($y$ direction), is denoted by $-\lambda_x$ ($-\lambda_y$), and the $\lambda_\nu^\dagger(m' - n, n)$ for $m'$, which is one of four basic rectangles involving the site being considered as a vertex, is denoted by $-\lambda'$. Then we have $-(2\lambda_x + 2\lambda_y + 4\lambda')s_z$ for $\Lambda(m)$ and

$$\rho^{(1)}(s) = \exp\left\{ \beta\left[ F^{(1)} + (h + 2\lambda_x + 2\lambda_y + 4\lambda')s_z \right] \right\} \tag{7.2}$$

where $F^{(1)}$ denotes $F(m)$ for this case.

We next consider a pair consisting of a site and one of its nearest neighbor sites in the $x$ direction, for $m$. We express the spin variables for the two sites as $s$ and $s'$. $\rho(m)$ for this case is denoted by $\rho_x^{(2)}(s, s')$. $H(m)$ is $-h(s_z + s_z') - J_x s \cdot s'$. In writing $\Lambda(m)$ in (4.9), $n$ is either one of the two sites consitituting $m$, or $m$ itself. When $n$ is the site for which the spin variable is $s$, we have only terms of $Q_\nu^\dagger(n) = s_z$; $m'$ for this case are all those occurring in the previous case where $m = n$ is a site, excluding $m$ itself, and we have $-(\lambda_x + 2\lambda_y + 4\lambda')s_z$. When $n$ is the other site, we have $-(\lambda_x + 2\lambda_y + 4\lambda')s_z'$. When $n$ is $m$ itself, the $Q_\nu(n)$ which appear are $s_z s_z'$ and $s \cdot s'$. $m'$ are two basic rectangles involving both sites of $m$ as vertices. Writing $\lambda(m' - n, n)$ for each rectangle as $-\lambda_x''$ and $-\lambda_x'''$, respectively, we have $-2\lambda_x'' s_z s_z' - 2\lambda_x''' s \cdot s'$ for $\Lambda(m)$. As a result we have

$$\rho_x^{(2)}(s, s') = \exp\left\{ \beta\left[ F_x^{(2)} + (h + \lambda_x + 2\lambda_y + 4\lambda')(s_z + s_z') + 2\lambda_x'' s_z s_z' + (J_x + 2\lambda_x''')s \cdot s' \right] \right\} \tag{7.3}$$

where $F_x^{(2)}$ denotes $F(m)$ for this case. In a similar way, for a pair of

nearest neighbor sites in the $y$ direction, we have

$$\rho_y^{(2)}(s,s') = \exp\Big\{\beta\Big[F_y^{(2)} + (h + 2\lambda_x + \lambda_y + 4\lambda')(s_z + s_z') + 2\lambda_y'' s_z s_z' + (J_y + 2\lambda_y''')s \cdot s'\Big]\Big\} \tag{7.4}$$

For a basic rectangle, we have

$$\begin{aligned}\rho^{(4)}(s,s',s'',s''') = \exp\Big\{\beta\Big[&F^{(4)} + (h + \lambda_x + \lambda_y + 3\lambda')(s_z + s_z' + s_z'' + s_z''') \\ &+ \lambda_x''(s_z s_z' + s_z'' s_z''') + \lambda_y''(s_z s_z''' + s_z' s_z'') \\ &+ (J_x + \lambda_x''')(s \cdot s' + s'' \cdot s''') \\ &+ (J_y + \lambda_y''')(s \cdot s''' + s' \cdot s'')\Big]\Big\}\end{aligned} \tag{7.5}$$

where $F^{(4)}$ is $F(m)$ for the case that $m$ is the basic rectangle.

$F^{(1)}$, $F_x^{(2)}$, $F_y^{(2)}$ and $F^{(4)}$ are determined by the normalization (2.6) for $\rho^{(1)}$, $\rho_x^{(2)}$, $\rho_y^{(2)}$ and $\rho^{(4)}$:

$$1 = \mathrm{Tr}\,\rho^{(1)}(s) = \mathrm{Tr}\,\rho_x^{(2)}(s,s') = \mathrm{Tr}\,\rho_y^{(2)}(s,s') = \mathrm{Tr}\,\rho^{(4)}(s,s's'',s''') \tag{7.6}$$

where Tr denotes the trace taken by the variables occurring in the respective operands. The effective fields $\lambda_x$, $\lambda_y$ and $\lambda'$ are determined by the consistency of the averages of $s_z$:

$$\mathrm{Tr}\,s_z\rho^{(1)}(s) = \mathrm{Tr}\,s_z\rho_x^{(2)}(s,s') = \mathrm{Tr}\,s_z\rho_y^{(2)}(s,s') = \mathrm{Tr}\,s_z\rho^{(4)}(s,s',s'',s''') \tag{7.7}$$

The effective interactions $\lambda_x''$ and $\lambda_x'''$ are determined by the consistency of the averages of $s_z s_z'$ and $s \cdot s'$:

$$\mathrm{Tr}\,s_z s_z'\rho_x^{(2)}(s,s') = \mathrm{Tr}\,s_z s_z'\rho^{(4)}(s,s',s'',s''') \tag{7.8}$$

$$\mathrm{Tr}\,s \cdot s'\rho_x^{(2)}(s,s') = \mathrm{Tr}\,s \cdot s'\rho^{(4)}(s,s',s'',s''') \tag{7.9}$$

and $\lambda_y''$ and $\lambda_y'''$ by

$$\mathrm{Tr}\,s_z s_z'''\rho_y^{(2)}(s,s''') = \mathrm{Tr}\,s_z s_z'''\rho^{(4)}(s,s',s'',s''') \tag{7.10}$$

$$\mathrm{Tr}\,s \cdot s'''\rho_y^{(2)}(s,s''') = \mathrm{Tr}\,s \cdot s'''\rho^{(4)}(s,s',s'',s''') \tag{7.11}$$

We shall write $f^\dagger(n)$ by $f^{(1)}$, $f_x^{(2)}$, $f_y^{(2)}$ and $f^{(4)}$, when $n$ is a site, a pair of nearest neighbors, one in the $x$ direction and one in the $y$ direction, and a basic rectangle, respectively. Then (4.8) reads

$$\begin{gathered}F^{(1)} = f^{(1)}, \qquad F_x^{(2)} = 2f^{(1)} + f_x^{(2)}, \qquad F_y^{(2)} = 2f^{(1)} + f_y^{(2)} \\ F^{(4)} = 4f^{(1)} + 2f_x^{(2)} + 2f_y^{(2)} + f^{(4)}\end{gathered} \tag{7.12}$$

and then, by (4.10), the free energy per site is given by

$$F/L = F^{(1)} + \left(F_x^{(2)} - 2F^{(1)}\right) + \left(F_y^{(2)} - 2F^{(1)}\right) + \left(F^{(4)} - 2F_x^{(2)} - 2F_y^{(2)} + 4F^{(1)}\right) \tag{7.13}$$

If $F^{(1)}$, $F_x^{(2)}$, $F_y^{(2)}$, and $F^{(4)}$ are calculated as a function of the effective fields and effective interactions by using (7.2)–(7.5) and (7.6), but not using (7.7)–(7.11), they can be determined by the stationariness of (7.13). In place of (7.7)–(7.11), we can also write the conditions of reducibility:

$$\begin{gathered} \rho^{(1)}(s) = \mathrm{tr}_{s'}\rho_x^{(2)}(s,s'), \qquad \rho^{(1)}(s) = \mathrm{tr}_{s'}\rho_y^{(2)}(s,s') \\ \rho_x^{(2)}(s,s') = \mathrm{tr}_{s'',s'''}\rho^{(4)}(s,s',s'',s''') \\ \rho_y^{(2)}(s,s''') = \mathrm{tr}_{s',s''}\rho^{(4)}(s,s',s'',s''') \end{gathered} \tag{7.14}$$

where subscripts following tr denote the variables with respect to which the trace is to be taken. In fact, (7.7)–(7.11) are a set of independent relations equivalent to the set (7.14).

If the formulations of Ref. 4 were adopted, $4\lambda'$ in (7.2), $4\lambda'$ in (7.3), $4\lambda'$ in (7.4), and $3\lambda'$ in (7.5) would be replaced by 0, $2\lambda_x'$, $2\lambda_y'$ and $\lambda_x' + \lambda_y'$, respectively. The effective fields in (7.2)–(7.5) would then be expressed in terms of three linear combinations $\lambda_x + \lambda_y$, $-\lambda_x + 2\lambda_x'$, and $-\lambda_y + 2\lambda_y'$; these are determined uniquely by the conditions (7.14), but $\lambda_x$, $\lambda_y$, $\lambda_x'$ and $\lambda_y'$ can all not be determined.

We considered the rectangular lattice. If the lattice is square and $J_x = J_y$, then we have four parameters $\lambda = \lambda_x = \lambda_y$, $\lambda'$, $\lambda'' = \lambda_x'' = \lambda_y''$, and $\lambda''' = \lambda_x''' = \lambda_y'''$ in the present formulation. The number of parameters in this case is the same also in the previous formulation.[4]

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