Generalized Ashkin-Teller model on the Bethe lattice

V. M. Rozenbaum,[1,2,*] A. N. Morozov,[2] and S. H. Lin[1]
[1]*Institute of Atomic and Molecular Sciences, Academia Sinica, P. O. Box 23-166, Taipei, Taiwan, Republic of China*
[2]*Institute of Surface Chemistry, National Academy of Sciences of Ukraine, Generala Naumova str. 17, Kiev, 03164, Ukraine*
(Received 16 December 2004; published 23 May 2005)

A generalized Ashkin-Teller model is considered that includes both biquadratic and opposite in sign bilinear interactions between two Ising subsystems, σ and s, along horizontal and vertical bonds on the Bethe lattice with the coordination number 4 (interactions of this kind are typical of adsorbed lattice systems characterized by dipolelike intermolecular forces and a strong azimuthal angular dependence of the C_4-symmetrical adsorption potential). The exact solutions found in the framework of this model: (*i*) determine the second-order phase transitions between paraphase I with $\langle\sigma\rangle=\langle s\rangle=\langle\sigma s\rangle=0$ and two ordered phases, phase II with $\langle\sigma\rangle=\langle s\rangle\neq 0$, $\langle\sigma s\rangle\neq 0$, and phase III with $\langle\sigma s\rangle\neq 0$ at $\langle\sigma\rangle=\langle s\rangle=0$ and (*ii*) specify the conditions for the conversion of second-order to first-order transitions. With regard to these solutions, the phase diagrams are constructed for K_1, K_2, K_4, where $K_i=J_i/k_BT$, J_1 is the interaction constant between σ-σ and s-s spin subsystems, J_2 is the constant of bilinear fluctuation σ-s interactions, J_4 is the constant of biquadratic σ-s interactions, k_B is the Boltzmann constant, and T is the absolute temperature. First-order transitions are detected numerically by comparing the free energies of the phases concerned. It is shown that phase II is gradually replaced by phases I and III with rising J_2 and vanishes at all if $J_2=J_1$.

DOI: 10.1103/PhysRevB.71.195411 PACS number(s): 68.35.Rh, 64.60.Cn, 05.50+q

I. INTRODUCTION

Among planar lattice models involved in statistical physics, those admitting exact solutions[1] are of most significance in the treatment of phase transitions in various realistic systems, e.g., two-dimensional antiferromagnets,[2] artificial two-dimensional lattices of ferromagnetic nanoparticles,[3] adsorbed molecular monolayers,[4,5] etc. The models implying four states of a particle at a lattice site are exemplified by the widely employed Ashkin-Teller model[6] and the spin-3/2 Ising model. These two are, in essence, equivalent (accurate to the number of included interactions between spins 3/2 and the restrictions imposed on the corresponding interaction constants), which makes the results obtained for either model valid for both of them.[7,8]

To describe orientational phase transitions in the systems with essentially anisotropic multipole Coulomb interactions, a more detailed study on anisotropic models was necessary. Thus, the phase transition on a square lattice of dipoles with four possible orientations along the square diagonals was simulated by a dipole short-range model reducible to the exactly soluble anisotropic Ising model.[9] A more complicated situation emerges if long molecular axes can have four orientations along the square lattice axes, since in this case the Ising subsystems (σ and s) are involved in opposite in sign bilinear interactions along the horizontal and vertical lattice bonds, so-called fluctuation interactions. These interactions can result in a new type of orientational ordering, viz., a preferential direction of long molecular axes in the absence of spontaneous polarization.[10] Phase transitions in the model with fluctuation interactions on a square lattice and on the Bethe lattice with the coordination number 4 were analyzed previously.[11] A generalized Ashkin-Teller model was introduced[12] in which the anisotropic bilinear interactions along with isotropic biquadratic interactions were included. This model is equivalent to the most general formulation of the anisotropic spin-3/2 model and admits, at a certain value of the fluctuation interaction parameter, an exact analytical solution for a square lattice.[12]

Like the conventional Ashkin-Teller model, its generalized analog admits no exact analytical solution throughout the variation range of the spin interaction parameters. As the self-consistent field approximation does not suffice to describe the fluctuation interactions, it is appropriate to invoke the corresponding model on the Bethe lattice. According to the known approach of Baxter,[1] the solutions obtained for this lattice can be regarded as exact ones; moreover, they provide a qualitatively correct description of phase transitions.[13] Here we present an exact analytical solution of the generalized Ashkin-Teller model which determines second-order phase transitions on the Bethe lattice with the coordination number 4 and specifies the conditions for the conversion of second-order to first-order transitions. Starting from the analytical solution as well as a numerical description of first-order transitions, a relevant phase-transition diagram is constructed.

II. GENERAL PROPERTIES OF THE MODEL

The Hamiltonian of the generalized Ashkin-Teller model with fluctuation interactions on a square lattice appears as follows:[12]

$$H=\sum_{mn}\big[-J_1(\sigma_{mn}\sigma_{m+1,n}+s_{mn}s_{m+1,n}+\sigma_{mn}\sigma_{m,n+1}+s_{mn}s_{m,n+1}) \\ -J_2(\sigma_{mn}s_{m+1,n}+s_{mn}\sigma_{m+1,n}-\sigma_{mn}s_{m,n+1}-s_{mn}\sigma_{m,n+1}) \\ -J_4(\sigma_{mn}s_{mn}\sigma_{m+1,n}s_{m+1,n}+\sigma_{mn}s_{mn}\sigma_{m,n+1}s_{m,n+1})\big]. \quad (1)$$

At $0\leqslant J_2\leqslant J_1$, the ground state energies and the corresponding spin distributions over the sites of a square lattice are specified by the relations

$$H_0 = \begin{cases} N(-4J_1 - 2J_4), & \sigma_{mn} = s_{mn} = 1, \quad J_4 > -J_1; \\ 2NJ_4, & \sigma_{mn}s_{mn} = (-1)^{m+n}, \quad J_4 < -J_1. \end{cases} \quad (2)$$

These states are degenerate in the interaction constant J_2. Note that the degeneracy occurs at an arbitrary J_1 to J_2 ratio. For instance, at $0 \leqslant J_1 \leqslant J_2$ the parameters J_1 and J_2 interchange, so that the degeneracy in J_1 results. If the interaction constants J_1 and J_2 have arbitrary signs, then the one with a larger absolute magnitude competes with $-J_4(J_4<0)$ in governing the ground state structure, whereas the other represents the degeneracy parameter. It is clear that the spin variables can be redesignated so that each of the resulting phase regions is describable by Hamiltonian (1) with the substitution $J_1 \leftrightarrow J_2$ or/and sign reversal for J_1 and J_2. Hence the statistical properties of all the phase regions are the same and one can restrict consideration to the region $0 \leqslant J_2 \leqslant J_1$ without loss of generality.

Some features of the phase diagram in terms of the variables $K_i = J_i / k_B T$, $i=1,2,4$ (k_B is the Boltzmann constant and T is the absolute temperature), are easily revealed from a number of limiting cases. At $K_2=0$, Hamiltonian (1) corresponds to the Ashkin-Teller model with the well-known phase diagram.[1] At $K_4=0$, the problem is reduced to the thoroughly studied case[11] of two interacting Ising sublattices with fluctuation interactions. As in the Ashkin-Teller model, the satisfied inequalities $0 \leqslant K_2 \leqslant K_1 \ll |K_4|$ imply that the system can be treated in terms of Ising solutions. Thus, the second-order phase transition from the disordered state $\langle\sigma\rangle = \langle s\rangle = \langle\sigma s\rangle = 0$ (phase I) to a phase with the nonzero average values of $\langle\sigma s\rangle$ at $\langle\sigma s\rangle = \langle s\rangle = 0$ (phase III) takes place if $K_4 = \pm K_{\mathrm{Ising}}$, where $K_{\mathrm{Ising}} = (1/2)\ln(1+\sqrt{2})$ for a square lattice and $K_{\mathrm{Ising}} = (1/2)\ln 2$ for the Bethe lattice with the coordination number 4. Interesting limiting peculiarities found at $K_4 \gg 1$ for the transition from phase III to phase II (with $\langle\sigma\rangle = \langle s\rangle > 0$) follow from Hamiltonian (1) which at $s_{mn} = \sigma_{mn}$ is reduced to the Hamiltonian of the Ising system with the different interaction constants along horizontal and vertical bonds:

$$H = \sum_{mn} [-2(J_1 + J_2)\sigma_{mn}\sigma_{m+1,n} - 2(J_1 - J_2)\sigma_{mn}\sigma_{m,n+1} - 2J_4]. \quad (3)$$

The phase transition temperature is therefore given by the following respective equations for a square lattice and for the Bethe lattice: $\sinh 4(K_1+K_2)\sinh 4(K_1-K_2)=1$ and $\exp[-4(K_1+K_2)]+\exp[-4(K_1-K_2)]=1$. At $J_2 \to J_1$, this temperature approaches zero by the logarithmic law which for the Bethe lattice assumes the form

$$T_{\text{II-III}} \approx \frac{8J_1}{\ln[T_{\text{II-III}}/4(J_1 - J_2)]}, \quad J_2 \to J_1. \quad (4)$$

The special case of $J_2 = J_1$ enables an exact analytical solution to be obtained, since the system turns quasi-one-dimensional and the partition function for either of the lattices considered is representable as[11,12]

$$Z = 2^N (\cosh 4K_1)^{N/2} Z_{\mathrm{Ising}}(\tilde{K}), \quad \tilde{K} = \tilde{K}_1 + K_4,$$
$$\tilde{K}_1 = \tfrac{1}{4}\ln(\cosh 4K_1). \quad (5)$$

Here $Z_{\mathrm{Ising}}(\tilde{K})$ designates the partition function for a two-dimensional Ising system with the effective Hamiltonian

$$H_{\mathrm{eff}} = -\tilde{J}\sum_{mn} (\tau_{mn}\tau_{m+1,n} + \tau_{mn}\tau_{m,n+1}), \quad \tilde{J} = T\tilde{K}, \quad (6)$$

in which $\tau_{mn} = \sigma_{mn}s_{mn}$ and the temperature-dependent interaction constant $\tilde{J}$ describes the thermodynamically averaged interaction of two neighboring σ spins. At $\tilde{J}>0$, the transition from phase I to phase III characterized by ferromagnetic ordering ($\langle\tau\rangle > 0$) is specified by the equation $\tilde{K} = K_{\mathrm{Ising}}$, which for the Bethe lattice with the coordination number 4 transforms to

$$\cosh 4K_1 = 4\exp(-4K_4). \quad (7)$$

At $\tilde{J}<0$, phase III suggests antiferromagnetic ordering ($\langle\tau_{mn}\rangle \propto (-1)^{m+n}$), so that $\tilde{K} = -K_{\mathrm{Ising}}$ and

$$\cosh 4K_1 = (1/4)\exp(-4K_4). \quad (8)$$

III. SOLUTION FOR THE BETHE LATTICE

The partition function corresponding to Hamiltonian (1) on a Cayley tree with the coordination number 4 can be written as follows:

$$Z(N) = \sum_{i=1}^{4} x_i^2(N) y_i^2(N), \quad (9)$$

where the values $x_i(N)$ and $y_i(N)$ are determined for the so-called central node of the tree (which is surrounded by N shells and lies farthest from the tree leaves where $N=0$) by the system of recurrent equations

$$x_i(N) = \sum_{j=1}^{4} \Lambda_{ij}^{(x)} x_j(N-1) y_j^2(N-1),$$
$$y_i(N) = \sum_{j=1}^{4} \Lambda_{ij}^{(y)} y_j(N-1) x_j^2(N-1). \quad (10)$$

Here, the indices i, $j=1,2,3,4$ label the following values assumed by the pairs of spin variables σ and s: $+1,+1$; $-1,-1$; $+1,-1$; $-1,+1$. The 4×4 matrices $\Lambda^{(x)}$ and $\Lambda^{(y)}$ have the block structure:

$$\Lambda^{(x)}=\begin{pmatrix}A & C\\ C & B\end{pmatrix},\quad \Lambda^{(y)}=\begin{pmatrix}B & C\\ C & A\end{pmatrix},$$

$$A=\begin{pmatrix}e^{2(K_1+K_2)+K_4} & e^{-2(K_1+K_2)+K_4}\\ e^{-2(K_1+K_2)+K_4} & e^{2(K_1+K_2)+K_4}\end{pmatrix}, \tag{11}$$

$$B=\begin{pmatrix}e^{2(K_1-K_2)+K_4} & e^{-2(K_1-K_2)+K_4}\\ e^{-2(K_1-K_2)+K_4} & e^{2(K_1-K_2)+K_4}\end{pmatrix},\quad C=\begin{pmatrix}e^{-K_4} & e^{-K_4}\\ e^{-K_4} & e^{-K_4}\end{pmatrix},$$

where $K_i=J_i/T$ (T is the absolute temperature in energy units). The quantities $x_i(n)$ and $y_i(n)$ determine the average values of spin variables in each lattice site n:

$$\langle\sigma\rangle_n=Z^{-1}(n)\sum_{i=1}^{4}\sigma_i x_i^2(n)y_i^2(n),\quad \langle s\rangle_n=Z^{-1}(n)\sum_{i=1}^{4}s_i x_i^2(n)y_i^2(n),$$
$$\langle\sigma s\rangle_n=Z^{-1}(n)\sum_{i=1}^{4}\sigma_i s_i x_i^2(n)y_i^2(n). \tag{12}$$

A general formula was previously derived for the free energy of an arbitrary spin system on the Bethe lattice corresponding to an anisotropic Cayley tree with the coordination number q at $N\to\infty$.[11] Applying this result to the system with $q=4$, we arrive at the following expression for the free energy of the Bethe lattice per lattice site:

$$f_{Bethe}=T\ln Z(N). \tag{13}$$

Note that the above definition has a reversed sign as compared to the conventional formula relating the free energy to the partition function. The two relations are not, however, in conflict because the latter, if adapted to the Bethe lattice, includes the factor $(2-q)/2$ equal to -1 at $q=4$. The Bethe lattice differs from the corresponding Cayley tree in that its sites are all equivalently accurate to the ordering type, ferromagnetic or antiferromagnetic. In the former case, the quantities x_i and y_i are independent of N and obey the system of equations (10). This implies that recurrent equations (10) determine, in the limit $N\to\infty$, a stable point x_i, y_i which defines, in turn, the free energy (13). In the latter case, it is sufficient to distinguish between the nodes N and $N-1$ and to assume the nodes N and $N-2$ equivalent. Hence for the system of eight equations (10) in 16 unknowns, $x_i(N)$, $y_i(N)$ and $x_i(N-1)$, $y_i(N-1)$ should be supplemented by another eight equations of the same form, only with $N-1$ replaced for N and $x_i(N-2)=x_i(N)$, $y_i(N-2)=y_i(N)$. The two above-mentioned cases will be considered separately.

A. Ferromagnetic ordering ($K_1+K_4>0$)

It is appropriate to involve the eigenvalues of the matrices $\Lambda^{(x)}$ and $\Lambda^{(y)}$,

$$\lambda_1=a_1,\quad \lambda_2=b_1,\quad \lambda_{3,4}=\tfrac{1}{2}[a_2+b_2\mp c],$$
$$c=\sqrt{(a_2-b_2)^2+16\exp(-2K_4)}, \tag{14}$$

which are expressible in terms of the eigenvalues of the matrices A and B:

$$a_1=2\exp(K_4)\sinh 2(K_1+K_2),$$
$$a_2=2\exp(K_4)\cosh 2(K_1+K_2),$$
$$b_1=2\exp(K_4)\sinh 2(K_1-K_2),$$
$$b_2=2\exp(K_4)\cosh 2(K_1-K_2). \tag{15}$$

The eigenvectors of the matrices $\Lambda^{(x)}$ and $\Lambda^{(y)}$ are representable in a block form:

$$S^{(x)}=\begin{pmatrix}S_1 & S_3\\ S_2 & S_4\end{pmatrix},\quad S^{(y)}=\begin{pmatrix}S_2 & S_4\\ S_1 & S_3\end{pmatrix},$$

$$S_1=\begin{pmatrix}2^{-1/2} & 0\\ -2^{-1/2} & 0\end{pmatrix},\quad S_2=\begin{pmatrix}0 & 2^{-1/2}\\ 0 & -2^{-1/2}\end{pmatrix}, \tag{16}$$

$$S_{3,4}=\begin{pmatrix}\pm(c\exp(K_4)\gamma_{3,4})^{-1/2} & (c\exp(K_4)\gamma_{4,3})^{-1/2}\\ \pm(c\exp(K_4)\gamma_{3,4})^{-1/2} & (c\exp(K_4)\gamma_{4,3})^{-1/2}\end{pmatrix},$$

where

$$\gamma_{3,4}=\frac{\exp K_4}{4}[c\pm(a_2-b_2)],\quad \gamma_3\gamma_4=1. \tag{17}$$

For the case of ferromagnetic ordering, the quantities x_i and y_i in the limit $N\to\infty$ are independent of N and satisfy the system of equations (10), which, in view of relations (14)–(17), can be written as

$$\sum_{i=1}^{4}(1-\lambda_k y_i^2)S_{ik}^{(x)}x_i=0,$$
$$\sum_{i=1}^{4}(1-\lambda_k x_i^2)S_{ik}^{(y)}y_i=0,\quad k=1,2,3,4. \tag{18}$$

Introducing the following ratios for the variables x_i and y_i,

$$\xi_{ij}=\frac{x_i}{x_j},\quad \eta_{ij}=\frac{y_i}{y_j}, \tag{19}$$

we obtain the explicit form of Eqs. (18):

$$x_1^2=\frac{1-\eta_{12}}{\lambda_2(\xi_{21}^2-\eta_{12})}=\frac{1-\eta_{34}}{\lambda_1(\xi_{43}^2-\eta_{34})\xi_{31}^2}$$
$$=\frac{1+\eta_{34}-\gamma_3(1+\eta_{12})\eta_{24}}{\lambda_3[(\xi_{43}^2+\eta_{34})\xi_{31}^2-\gamma_3(\xi_{21}^2+\eta_{12})\eta_{24}]}$$
$$=\frac{1+\eta_{34}+\gamma_4(1+\eta_{12})\eta_{24}}{\lambda_4[(\xi_{43}^2+\eta_{34})\xi_{31}^2+\gamma_4(\xi_{21}^2+\eta_{12})\eta_{24}]},$$
$$y_4^2=\frac{1-\xi_{43}}{\lambda_2(\eta_{34}^2-\xi_{43})}=\frac{1-\xi_{21}}{\lambda_1(\eta_{12}^2-\xi_{21})\eta_{24}^2}$$
$$=\frac{1+\xi_{21}-\gamma_3(1+\xi_{43})\xi_{31}}{\lambda_3[(\eta_{12}^2+\xi_{21})\eta_{24}^2-\gamma_3(\eta_{34}^2+\xi_{43})\xi_{31}]}$$
$$=\frac{1+\xi_{21}+\gamma_4(1+\xi_{43})\xi_{31}}{\lambda_4[(\eta_{12}^2+\xi_{21})\eta_{24}^2+\gamma_4(\eta_{34}^2+\xi_{43})\xi_{31}]}. \tag{20}$$

In terms of variables (19), the average values of spin variables (12) at each lattice site appear as

$$\langle\sigma\rangle=\frac{(\eta_{12}^2-\xi_{21}^2)\eta_{24}^2+(\eta_{34}^2-\xi_{43}^2)\xi_{31}^2}{(\eta_{12}^2+\xi_{21}^2)\eta_{24}^2+(\eta_{34}^2+\xi_{43}^2)\xi_{31}^2},$$

$$\langle s\rangle=\frac{(\eta_{12}^2-\xi_{21}^2)\eta_{24}^2-(\eta_{34}^2-\xi_{43}^2)\xi_{31}^2}{(\eta_{12}^2+\xi_{21}^2)\eta_{24}^2+(\eta_{34}^2+\xi_{43}^2)\xi_{31}^2}, \qquad (21)$$

$$\langle\sigma s\rangle=\frac{(\eta_{12}^2+\xi_{21}^2)\eta_{24}^2-(\eta_{34}^2+\xi_{43}^2)\xi_{31}^2}{(\eta_{12}^2+\xi_{21}^2)\eta_{24}^2+(\eta_{34}^2+\xi_{43}^2)\xi_{31}^2}.$$

Note that the symmetry of the problem leads to the equality $\langle\sigma\rangle=\pm\langle s\rangle$. One can deem, without loss of generality, that $\langle\sigma\rangle=\langle s\rangle$ and restrict the consideration to the range of values $\langle\sigma\rangle=\langle s\rangle\geqslant 0$. Then it follows from (21) that $\eta_{34}=\xi_{43}$. The condition $\langle\sigma\rangle=\langle s\rangle=0$ is met with the proviso that the equality $\eta_{12}=\xi_{21}$ holds. Since each fraction in Eq. (20) should be positive, the equality $\eta_{34}=\xi_{43}$ implies that $\eta_{34}=\xi_{43}=1$, whereas the quantities η_{12} and ξ_{21} enter into the chain of inequalities $0<\xi_{21}\leqslant 1\leqslant\eta_{12}$. At $\xi_{21}=\eta_{12}=1$ we have $\langle\sigma\rangle=\langle s\rangle=0$. Thus, the initial system of eight equations (18) in eight unknowns x_i, y_i $(i=1,2,3,4)$ is reduced to the system of four equations in the following unknowns:

$$\rho_1=\xi_{21},\quad \rho_2=\eta_{12},\quad \zeta_1=\frac{2a_2}{1+\rho_1}\xi_{31},\quad \zeta_2=\frac{a_2}{2}(1+\rho_2)\eta_{24}. \qquad (22)$$

Algebraic manipulation of Eqs. (20) results in the convenient representation of the four equations:

$$4\exp(-2K_4)\zeta_{1,2}[r+2\exp(-K_4)(\nu_1\nu_2-1)\ \zeta_{1,2}-\nu_1\nu_2\zeta_{1,2}^2)]^2 - \nu_{2,1}[\zeta_{1,2}-2\exp(-K_4)][r-2\exp(-K_4)\zeta_{1,2}](r - \nu_{1,2}\zeta_{1,2}^2)^2=0, \qquad (23)$$

$$\mu_1\equiv\frac{(1+\rho_2)(\rho_1^2-\rho_2)}{(1-\rho_2)(\rho_1^2+\rho_2)}=\frac{\lambda_3\lambda_4}{a_2\lambda_2}\frac{\zeta_2}{\zeta_2-2\exp(-K_4)},$$

$$\mu_2\equiv\frac{(1+\rho_1)(\rho_2^2-\rho_1)}{(1-\rho_1)(\rho_2^2+\rho_1)}=\frac{\lambda_3\lambda_4}{\lambda_1}\frac{a_2}{r-2\zeta_1\exp(-K_4)}, \qquad (24)$$

with $2\exp(-K_4)\leqslant\zeta_{1,2}\leqslant r\exp(K_4)/2$ and the notation

$$r\equiv a_2b_2,\quad \nu_1\equiv\frac{(1+\rho_1)^2(1+\rho_2)}{4(\rho_1^2+\rho_2)},\quad \nu_2\equiv\frac{4(\rho_2^2+\rho_1)}{(1+\rho_2)^2(1+\rho_1)}. \qquad (25)$$

First we consider solutions with $\rho_1=\rho_2=1$ that correspond to the case $\langle\sigma\rangle=\langle s\rangle=0$. For them, we have $\nu_1=\nu_2=1$ and Eqs. (23) simplified as follows:

$$(r-\zeta_{1,2}^2)^2[2(\zeta_{1,2}^2+r)\exp(-K_4)-r\zeta_{1,2}]=0. \qquad (26)$$

At $r\leqslant 16\exp(-2K_4)$, the only possible solution is

$$\zeta_1=\zeta_2=r^{1/2}. \qquad (27)$$

By virtue of equality $\eta_{24}=\xi_{31}$, this solution describes the state with $\langle\sigma s\rangle=0$ [see Eqs. (21)]. At $r>16\exp(-2K_4)$, another solution with $\zeta_2>\zeta_1$ arises:

$$\zeta_{2,1}=\frac{\exp(K_4)}{4}r^{1/2}\{r^{1/2}\pm[r-16\exp(-2K_4)]^{1/2}\}. \qquad (28)$$

It suggests the state with $\langle\sigma s\rangle>0$:

$$\langle\sigma s\rangle=\frac{r^{1/2}[r-16\exp(-2K_4)]^{1/2}}{r-8\exp(-2K_4)}. \qquad (29)$$

The states with $\langle\sigma s\rangle=0$ and $\langle\sigma s\rangle>0$ at $\langle\sigma\rangle=\langle s\rangle=0$ will be referred to as phases I and III (phase II will identify the state with $\langle\sigma\rangle=\langle s\rangle>0$). The continuous second-order phase transitions I–III are characterized by the equation $r=16\exp(-2K_4)$, which is equivalent to the following:

$$\cosh(4K_1)+\cosh(4K_2)=8\exp(-4K_4). \qquad (30)$$

At $K_2=K_1$ Eq. (30) transforms to (7) and at $K_4\gg K_1$, K_2 the I–III transition is approximately describable by the Ising model on the Bethe lattice with the transition temperature $T_{\text{I–III}}\approx 2J_4/\ln 2$.[1] In the vicinity of the transition I–III within phase III, the quantity $\langle\sigma s\rangle$ tends to zero with the critical exponent 1/2 [see formula (29)], which is consistent with the temperature dependence of the order parameter in the mean-field theory.

We now turn to the analysis of the solutions with $\rho_1<1<\rho_2$ corresponding to the case $\langle\sigma\rangle=\langle s\rangle>0$ (phase II). Inferring that the transitions I–II [at $r\leqslant 16\exp(-2K_4)$] and III–II [at $r>16\exp(-2K_4)$] are of the second order, the variables ρ_1 and ρ_2 should continuously approach unity in the vicinity of these transitions within phase II. To derive equations relevant to the second-order phase transitions I–II or III–II, it is therefore necessary to consider the system of equations (23) and (24) in the limit ρ_1, $\rho_2\to 1$. In so doing, the variables ρ_1 and ρ_2 are conveniently expressed in terms of μ_1 and μ_2 using Eqs. (24):

$$\rho_{1,2}=\frac{2(\mu_{1,2}+1)^2(\mu_{2,1}^2+1)-(\mu_{1,2}-1)^2(\mu_{2,1}+1)^2\mp\sqrt{D}}{2(\mu_{1,2}+1)^2(\mu_{2,1}^2-1)}, \qquad (31)$$

$$D=(-1+\mu_1+\mu_2+3\mu_1\mu_2)(1+3\mu_1-\mu_2+\mu_1\mu_2)(1-\mu_1 + 3\mu_2+\mu_1\mu_2)(3+\mu_1+\mu_2-\mu_1\mu_2).$$

The limit of interest, $\rho_1,\rho_2\to 1$, corresponds to the region

$$t\equiv 3+\mu_1+\mu_2-\mu_1\mu_2\geqslant 0,\quad \mu_1\geqslant 1,\quad \mu_2\geqslant 1. \qquad (32)$$

Indeed, at $t\to 0$ we obtain, accurate to the terms of the order t,

$$\rho_1\approx 1-p\varepsilon+\tfrac{1}{2}p^2\varepsilon^2,\quad \rho_2\approx 1+\varepsilon+\tfrac{1}{2}\varepsilon^2,\quad \varepsilon\ll 1, \qquad (33)$$

with the notation

$$\varepsilon \equiv \frac{\sqrt{2t}}{\mu_1 + 1}, \quad p \equiv \frac{1}{2}(\mu_1 - 1). \tag{34}$$

Substituting power series (33) into expressions (25), we arrive, with the same accuracy, to the following relations:

$$\nu_1 \approx 1 - \tfrac{1}{4}p(p+2)\varepsilon^2, \quad \nu_2 \approx 1 + \tfrac{1}{4}(1+2p)\varepsilon^2. \tag{35}$$

The system of equations (23) can now be solved approximately with respect to the variables ζ_1 and ζ_2; substituting the solutions found into relations (24) affords the values of the variables μ_1 and μ_2. The latter enable, with definitions (32) and (34), a closed equation in the small parameter ε to be written. In a zeroth-order approximation in ε, the system of equations (23) has two solutions (27) and (28), depending on the parameter r. Hence it is appropriate to separately consider the intervals $r \leqslant 16\exp(-2K_4)$ and $r > 16\exp(-2K_4)$ corresponding to the phase transitions I–II and III–II.

At $r \leqslant 16\exp(-2K_4)$ we are led to

$$\zeta_{1,2} \approx r^{1/2} - \frac{1}{2}\frac{r^{1/2} - 2\exp(-K_4)}{4 - r^{1/2}\exp(K_4)}\{2\nu'_{2,1} - [r^{1/2}\exp(K_4) - 2]\nu'_{1,2}\}\varepsilon^2,$$

$$\mu_{1,2} \approx f_{1,2}\left(1 \pm \frac{2\exp(-K_4)(\nu'_1 + \nu'_2) - r^{1/2}\nu'_{2,1}}{r^{1/2}[4 - r^{1/2}\exp(K_4)]}\varepsilon^2\right),$$

$$f_1 \equiv \frac{r^{1/2}[r^{1/2} + 2\exp(-K_4)]}{\lambda_2 a_2},$$

$$f_2 \equiv \frac{a_2[r^{1/2} + 2\exp(-K_4)]}{r^{1/2}\lambda_1}, \quad \nu'_{1,2} = \left(\frac{\partial \nu_{1,2}}{\partial \varepsilon^2}\right)_{\varepsilon=0}. \tag{36}$$

The solution of the equation in ε can be represented as follows:

$$\varepsilon^2 = \frac{2}{(f_1+1)^2(1-\kappa)}t, \tag{37}$$

$$\kappa = \frac{r^{1/2}[(1+2p)f_2 + p(p+2)f_1 + 3(1+4p+p^2)] + 2(1-p^2)(f_1 - f_2)\exp(-K_4)}{2r^{1/2}[4 - r^{1/2}\exp(K_4)](f_1+1)^2}. \tag{38}$$

The quantities t and p are determined by relations (32) and (34), with the values f_1 and f_2 from Eq. (36) substituted for μ_1 and μ_2. From solution (37) it follows that the second-order transition I–II occurs at

$$t = 3 + f_1 + f_2 - f_1 f_2 = 0, \tag{39}$$

if the coefficient κ falls within the range from 0 to 1. For instance, $\kappa=1$ at $J_4=0$ when $J_2/J_1=0.5633$, $T/J_1=2.4725$, and the second-order transitions I–II take place on the interval $0 \leqslant J_2/J_1 \leqslant 0.5633$, in accordance with previous results.[11] Substitution of ρ_1, ρ_2 from Eq. (33) and ζ_1, ζ_2 from Eq. (36) (in the form of power series in ε) into relations (21) provides, with regard to notation used in Eq. (22),

$$\langle\sigma\rangle = \frac{1}{2}(1+p)\varepsilon, \quad \langle\sigma s\rangle = \frac{1+4p+p^2}{4[4 - r^{1/2}\exp(K_4)]}\varepsilon^2. \tag{40}$$

From relations (32), (37), and (39) it follows that the parameter t is proportional to the temperature difference $T_c - T$ [T is the temperature within phase II; T_c is the temperature of the phase transition I–II satisfying Eq. (39)], and the parameter ε is proportional to $t^{1/2}$. As a result, the quantity $\langle\sigma\rangle$ in phase II in the vicinity of the I–II phase boundary approaches zero with the critical exponent 1/2, in accordance with the temperature dependence of the order parameter in the mean-field approximation. For the quantity $\langle\sigma s\rangle$, the corresponding critical exponent is equal to 1. At $J_2=J_4=0$ we have, in the limit $t\to 0$, $p=1$, $r^{1/2}=5/2$, $T_{\text{I–II}}=2J_1/\ln 2$, and $\langle\sigma s\rangle = \langle\sigma\rangle^2 = \varepsilon^2 = t/2$, where $t=16(1-2z)$, $z\equiv\exp(-2K_1)$. This result conforms to the Ising model on the Bethe lattice,[1] which implies the following temperature dependence for the averages of the statistically independent spins σ and s in the ordered phase: $\langle\sigma\rangle = (1-4z^2)^{1/2}/(1-2z^2)$.

We now turn to the analysis of the second-order transitions II–III occurring at $r > 16\exp(-2K_4)$. Relations (36) need to be rewritten accordingly:

$$\zeta_{1,2} = \zeta_{1,2}^{(\text{III})}\left(1 + 4\frac{r\nu'_{2,1} - 8(\nu'_1 + \nu'_2)\exp(-2K_4)}{r[16 - r\exp(2K_4)]}\varepsilon^2\right),$$

$$\mu_{1,2} = f_{1,2}\left(1 \mp 2[\zeta_1^{(\text{III})} - 2\exp(-K_4)] \times \frac{r\nu'_{1,2} - 8(\nu'_1 + \nu'_2)\exp(-2K_4)}{r[16 - r\exp(2K_4)]}\varepsilon^2\right),$$

$$f_1 \equiv \frac{[r - 4\exp(-2K_4)]\zeta_1^{(\text{III})}}{2\lambda_2 a_2\exp(-K_4)},$$

$$f_2 \equiv \frac{a_2[r - 4\exp(-2K_4)]}{2\lambda_1\zeta_2^{(\text{III})}\exp(-K_4)}, \quad \nu'_{1,2} = \left(\frac{\partial \nu_{1,2}}{\partial \varepsilon^2}\right)_{\varepsilon=0}, \tag{41}$$

where $\zeta_{2,1}^{(\text{III})}$ correspond to the values specified by Eq. (28) for phase III. Equation (37) retains the same form, with the value f_1 defined as in Eq. (41) and the parameter κ expressed as

$$\kappa = \frac{\zeta_1^{(\mathrm{III})} - 2\exp(-K_4)}{r(f_1+1)^2\exp(K_4)} \frac{r[(1+2p)f_1 + p(p+2)f_2 + 3(1+4p+p^2)] - 8(1-p^2)(f_1-f_2)\exp(-2K_4)}{r - 16\exp(-2K_4)}. \tag{42}$$

The second-order transition II–III is realized subject to the same condition (39) if the value of the coefficient κ falls within the range from 0 to 1. The value $\kappa=1$ at $J_4=0$ is now found at the point with the coordinates $J_2/J_1=0.9683$, $T/J_1=1.7300$, and the above-mentioned transition occurs on the interval $0.9683 \leqslant J_2/J_1 \leqslant 1$. Note that the numerical values first obtained in Ref. 11 ($J_2/J_1=0.9590, T/J_1=1.7663$) are refined here via the correction of formulas (42) and (43).

At $r > 16\exp(-2K_4)$, relation (40) transforms to

$$\langle \sigma \rangle = \frac{1+p}{1+(\zeta_1^{(\mathrm{III})}/\zeta_2^{(\mathrm{III})})^2}\varepsilon, \tag{43}$$

$$\langle \sigma s \rangle - \langle \sigma s \rangle_{\mathrm{III}} = \frac{8(1+4p+p^2)}{[r\exp(2K_4)-8][r\exp(2K_4)-16]}\varepsilon^2, \tag{43}$$

where $\langle \sigma s \rangle_{\mathrm{III}}$ is determined by expression (29) for phase III. These order parameters have the same values of critical indices as in phase II at $r \leqslant 16\exp(-2K_4)$.

As the parameter J_2/J_1 approaches unity, the phase transition temperature goes to zero. At $J_2/J_1 \to 1$, Eq. (39) is simplified:

$$4(K_1 - K_2) \approx \exp(-8K_1)[2\exp(-8K_4)+1] \tag{44}$$

or

$$T_{\text{II-III}} \approx \frac{8J_1}{\ln[\gamma T_{\text{II-III}}/(J_1-J_2)]}, \quad \gamma = \frac{2\exp(-8K_4)+1}{4}, \quad J_2 \to J_1. \tag{45}$$

Equation (45) has the same form as the asymptotic equation in transition temperature in the two-dimensional Ising model for a square lattice with interactions along either horizontal or vertical bonds tending to zero. Such interactions are simulated in Eq. (45) by the quantity J_1-J_2. The difference between the two equations is confined to the coefficient values and results from the existence of two sublattices and the specificity of the model involved as well as from the fact that the fluctuation interactions are included to a different degree on the Bethe lattice and on a square lattice. In the limit $K_4 \to \infty$, Eq. (45) is reduced to Eq. (4) considered in Sec. II.

B. Antiferromagnetic ordering ($K_1+K_4<0$)

At $K_1+K_4<0$, the conventional Ashkin-Teller model is known to admit only two phases, phase I and antiferromagnetic phase III. The same is true for the generalized model. The condition for the absence of phase II appears as

$$\langle \sigma \rangle_n = \langle s \rangle_n = 0 \quad (n = N, N-1). \tag{46}$$

This expression permits us to simplify the system of 16 equations in the unknowns $x_i(N)$, $y_i(N)$ and $x_i(N-1)$, $y_i(N-1)$, which was obtained from the initial system of eight equations (10) as indicated at the beginning of Sec. III. With Eqs. (12), the following relations are derived for ratios (19) of the above unknowns:

$$\xi_{12}(n) = \eta_{12}(n) = \xi_{34}(n) = \eta_{34}(n) = 1 \quad (n = N, N-1). \tag{47}$$

Then the system of equations (10) can be rewritten in terms of the variables specified by Eqs. (19):

$$\xi_{13}(N) = \frac{a\xi_{13}(N-1)\eta_{13}^2(N-1)+1}{\xi_{13}(N-1)\eta_{13}^2(N-1)+b}, \quad \eta_{13}(N) = \frac{b\xi_{13}^2(N-1)\eta_{13}(N-1)+1}{\xi_{13}^2(N-1)\eta_{13}(N-1)+a}, \tag{48}$$

where

$$a = \exp(2K_4)\cosh 2(K_1+K_2), \quad b = \exp(2K_4)\cosh 2(K_1-K_2). \tag{49}$$

In addition to Eqs. (48), one needs to solve another two equations of the same form, only with $N-1$ replaced for N, using the identity of the variables at the sites N and $N-2$. Of importance are the solutions which imply the nullified (phase I) or opposite in sign (phase III) average products of the spins s and σ at neighboring lattice sites, so that

$$\langle \sigma s \rangle_N = -\langle \sigma s \rangle_{N-1}. \tag{50}$$

Such a restriction corresponds to the antiferromagnetic ground state (2) at $K_1+K_4<0$. Then the following equality is valid:

$$\xi_{13}(N)\eta_{13}(N)\xi_{13}(N-1)\eta_{13}(N-1) = 1. \tag{51}$$

At $4ab \geqslant 1$, it admits a single solution:

$$\xi_{13}(N) = \xi_{13}(N-1) = \sqrt{\frac{a}{b}}, \quad \eta_{13}(N) = \eta_{13}(N-1) = \sqrt{\frac{b}{a}}, \tag{52}$$

which describes the state with $\langle \sigma s \rangle = 0$ (phase I). At $4ab<1$, an additional solution results:

$$\xi_{13}^{\pm}(N) = \frac{1}{\eta_{13}^{\mp}(N)} = \xi_{13}^{\mp}(N-1) = \frac{1}{\eta_{13}^{\pm}(N-1)} = \frac{1 \pm \sqrt{1-4ab}}{2b}, \tag{53}$$

which refers to the state with $\langle \sigma s \rangle \neq 0$ (phase III). Here the choice of signs dictates the signs of the average values given by Eq. (50). Inferring the average product of the spins s and σ to be positive at the central site, we arrive at

$$\langle \sigma s \rangle_N = \frac{\sqrt{1-4ab}}{1-2ab}, \quad 4ab \leq 1. \tag{54}$$

The second-order phase transition I–III is characterized by the equation $4ab=1$ which is equivalent to the following one:

$$\cosh(4K_1) + \cosh(4K_2) = (1/2)\exp(-4K_4). \tag{55}$$

At $K_2=K_1$ Eq. (55) is reduced to Eq. (8), whereas at $K_4 \geqslant K_1$, K_2 the transition I–III is roughly described by the Ising model on the Bethe lattice, with the temperature $T_{\text{I–III}} \approx -2J_4/\ln 2$.[1] In the vicinity of the transition I–III within phase III, the quantity $\langle \sigma s \rangle_N$ approaches zero with the critical exponent 1/2 [see formula (54)], thus conforming to the temperature dependence of the order parameter in the mean-field theory.

IV. PHASE DIAGRAM

Equations (30), (39), and (55) derived for the second-order transitions between phases I, II, and III correspond to certain surfaces in a three-dimensional space of the parameters K_1, K_2, and K_4. The conventional Ashkin-Teller model manipulates only two parameters, K_1 and K_4, and accordingly suggests a planar phase diagram. First we introduce a phase diagram for the generalized Ashkin-Teller model in the same coordinates, K_1 and K_4, and show a family of the curves corresponding to various K_2/K_1 ratios (see Fig. 1). The dashed curves representing the first-order transitions I–II were calculated by solving the system of equations (10) numerically and equating the free energies (13) of the phases concerned. At the points where $\kappa=1$, these lines have common tangents with those referring to the second-order phase transitions [see Eqs. (38) and (42)]. This result is in agreement with the properties of critical points between the lines of first- and second-order phase transitions in terms of the Landau theory.[14]

An alternative representation of the phase diagram in the coordinates K_1 and K_2 (see Fig. 2) was employed previously[10,11] in the analysis of the properties of pure fluctuation interactions, at $K_4=0$. The family of curves with the varied K_4/K_1 ratio demonstrates the effect caused by biquadratic interactions of the Ashkin-Teller model, if added to a system with pure fluctuation interactions.

The diagram regions with small values of K_1 and K_4 correspond to high temperatures and paraphase I. As the ratio K_2/K_1 rises, phase II and antiferromagnetic phase III are replaced by phase I. At the same time, both phase I and phase II give way to ferromagnetic phase III. In the limit $K_4 \to \infty$, phase II is forced out to infinity and, at $K_2=K_1$, it vanishes at all.

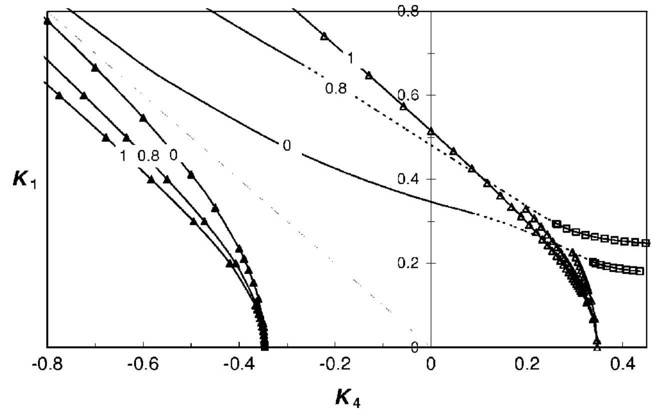

FIG. 1. The phase diagram in the coordinates K_1 and K_4 for the generalized Ashkin-Teller model on the Bethe lattice with the coordination number 4. The K_2/K_1 ratios are indicated near the curves. Solid and dashed lines respectively represent second-order and first-order transitions. Solid lines without markers separate phases I and II. Dashed lines separate phases I and II before crossing at the triple point (where three phases coexist) and become the boundaries between phases II and III after going through that point. Solid lines with squares separate phases II and III. Solid lines with empty triangles separate phases I and III. Solid lines with filled triangles separate phase I and antiferromagnetic phase III.

V. DISCUSSION AND CONCLUSIONS

Hamiltonian (1) of the generalized Ashkin-Teller model is introduced to account for orientational phase transitions in a lattice system of adsorbed molecules with quasinormal orientations.[15] The parameters of the model were estimated previously[10,11] for the 2×1 monolayer of CO molecules adsorbed on the NaCl(100) surface: $J_2 \approx 0.6J_1$, $J_4 \approx -0.2J_1$, $J_1 \approx 0.8$ meV. The Monte Carlo simulation performed with these parameter values provides the phase transition temperature within the experimentally observed temperature range 17.5–21.5 K.[16] Thus, the phase diagram of the generalized Ashkin-Teller model is helpful in the study of orientational behavior of adsorbates. It also affords a better understanding of phase transitions in the systems with fluctuation interactions. However, a three-parameter phase diagram on a

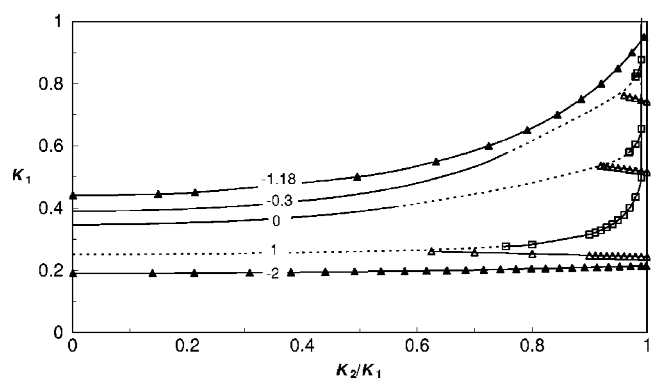

FIG. 2. The phase diagram in the coordinates K_1 and K_2/K_1 for the generalized Ashkin-Teller model on the Bethe lattice with the coordination number 4. The K_4/K_1 ratios are indicated near the curves. All designations are the same as in Fig. 1.

square lattice can be constructed only by the Monte Carlo numerical simulation, a laborious and time-consuming procedure. Here we report an analytical solution of the problem which is an exact one for the Bethe lattice with the coordination number 4 and also gives a qualitatively correct description of phase transitions on a square lattice.

The main result of this work is the construction of the phase diagrams depicted in Figs. 1 and 2. It is seen that the region occupied by phase II is replaced by phases I and III, as the constant J_2 increases, and phase II vanishes completely at $J_2 = J_1$. This inference conforms with the previous results gained for a square lattice.[12] The generalized Ashkin-Teller model provides a more penetrating insight into the behavior of a system with strong fluctuation interactions, when $J_2 \to J_1$. At $K_4 \gg 1$, the transition from phase III to phase II is a counterpart of the Ising-model transition in a system with different interaction constants along horizontal and vertical bonds. The interaction constants are simulated in our approach by the sum and the difference of the parameters J_1 and J_2. It is therefore evident that in the limit $J_2 \to J_1$, one of the Ising-model interaction constants tends to zero; hence the temperature of the transition II–III falls by the logarithmic law—see Eq. (4). If the parameter K_4 assumes an arbitrary positive value, there will be a change only in the insignificant factor γ in the argument of the logarithmic function, as seen from Eq. (45).

Generally, bilinear fluctuation interactions introduced into the Ashkin-Teller model resemble, to some extent, biquadratic interactions inherent in this approach. In addition to paraphase I ($\langle\sigma\rangle = \langle s\rangle = \langle\sigma s\rangle = 0$) and ordered phase II ($\langle\sigma\rangle, \langle s\rangle, \langle\sigma s\rangle \neq 0$), a new phase III ($\langle\sigma s\rangle \neq 0$ at $\langle\sigma\rangle = \langle s\rangle = 0$) emerges. Besides, the transitions I–II in a certain range of the interaction constant values represent first-order transitions. A basic distinctive feature of the fluctuation interactions is that their enhancement leads one of the spin subsystems becoming quasi-one-dimensional and causes the replacement of phase II by other phases.

ACKNOWLEDGMENTS

The authors thank Dr. M. L. Dekhtyar for her helpful comments on the manuscript. This work was supported by Academia Sinica. V.M.R. gratefully acknowledges the kind hospitality received from the Institute of Atomic and Molecular Sciences.

*E-mail: vrozen@mail.kar.net

[1] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982).
[2] C. L. Henley, Phys. Rev. Lett. **62**, 2056 (1989).
[3] S. A. Gusev, Yu. N. Nozdrin, M. V. Sapozhnikov, and A. A. Fraerman, Usp. Fiz. Nauk **170**, 331 (2000) [Phys. Usp. **43**, 288 (2000)].
[4] V. M. Rozenbaum, V. M. Ogenko, and A. A. Chuiko, Usp. Fiz. Nauk **161**(10), 79 (1991) [Sov. Phys. Usp. **34**, 883 (1991)].
[5] V. M. Rozenbaum and S. H. Lin, *Spectroscopy and Dynamics of Orientationally Structured Adsorbates* (World Scientific, Singapore, 2002).
[6] J. Ashkin and E. Teller, Phys. Rev. **64**, 178 (1943).
[7] T. Horiguchi and Y. Honda, Prog. Theor. Phys. **93**, 981 (1995).
[8] N. Sh. Izmailian, Pis'ma Zh. Eksp. Teor. Fiz. **63**, 270 (1996) [JETP Lett. **63**, 290 (1996)].
[9] V. M. Rozenbaum and V. M. Ogenko, Pis'ma Zh. Eksp. Teor. Fiz. **35**, 151 (1982) [JETP Lett. **35**, 184 (1982)].
[10] V. M. Rozenbaum and A. N. Morozov, Pis'ma Zh. Eksp. Teor. Fiz. **75**, 756 (2002) [JETP Lett. **75**, 631 (2002)].
[11] V. M. Rozenbaum, A. N. Morozov, and S. H. Lin, Phys. Rev. B **68**, 155405 (2003).
[12] V. M. Rozenbaum, Pis'ma Zh. Eksp. Teor. Fiz. **78**, 40 (2003) [JETP Lett. **78**, 34 (2003)].
[13] P. D. Gujrati, Phys. Rev. Lett. **74**, 809 (1995).
[14] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1980).
[15] V. M. Rozenbaum and S. H. Lin, J. Chem. Phys. **112**, 9083 (2000).
[16] J. Heidberg, M. Grunwald, M. Hustedt, and F. Traeger, Surf. Sci. **368**, 126 (1996).