Eur. Phys. J. D **12**, 311–322 (2000)

THE EUROPEAN
PHYSICAL JOURNAL D
EDP Sciences

Adatom diffusion on a square lattice. Theoretical and numerical studies

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Received 1st September 1998 and Received in final form 8 March 2000

Abstract. A two-dimensional lattice-gas model with square symmetry is investigated by using the real-space renormalization group (RSRG) approach with blocks of different size and symmetries. It has been shown that the precision of the method depends strongly not only on the number of sites in the block but also on its symmetry. In general, the accuracy of the method increases with the number of sites in the block. The minimal relative error in determining the critical values of the interaction parameters is equal to 0.13%. Using the RSRG method, we have explored phase diagrams of both a two-dimensional Ising spin model and of a square lattice gas with lateral interactions between adparticles. We also have investigated the influence of the attractive and repulsive interactions on both the thermodynamic properties of the lattice gas and the diffusion of adsorbed particles over surface. We have calculated adsorption isotherms and coverage dependences of the pair correlation function, isothermal susceptibility and the chemical diffusion coefficient. In addition, we have included in our analysis the interaction of the activated particle in the saddle point with its nearest neighbors. We have also used Monte Carlo (MC) technique to calculate these dependences. Despite the fact that both methods constitute very different approaches, the correspondence of the numerical data is surprisingly good. Therefore, we conclude that the RSRG approach can be applied to characterize the thermodynamic and kinetic properties of systems of particles with strong lateral interactions.

PACS. 64.60.Ak Renormalization-group, fractal, and percolation studies of phase transitions – 68.35.Rh Phase transitions and critical phenomena – 68.35.Fx Diffusion; interface formation

1 Introduction

The migration of adsorbates on solid surfaces plays an essential role in many physical and chemical processes such as adsorption, desorption, melting, roughening, crystal and film growth, catalysis and corrosion. Understanding surface diffusion is one of the keys to controlling these processes.

In recent years, the effects of lateral interactions on the chemical surface diffusion coefficient of adsorbed particles have been intensively investigated using many different theoretical methods applicable to critical phenomena [1–6]. It has been found that adparticle interactions can strongly influence surface diffusion, especially at low temperatures and in the close vicinity of phase transitions. It is intuitively expected that attractive interactions between adsorbed species inhibit the adparticle migration and thus slow down surface diffusion. In contrast, repulsive interactions are expected to accelerate surface diffusion. Despite their simplicity, these rules describe the qualitative behavior of surface diffusion processes for many systems. However, the most sophisticated methods are required for the description of surface diffusion in case of strong lateral interactions between adparticles which force the system to order below a critical temperature. The critical behavior of the tracer, jump and chemical diffusion coefficients has been discussed in the literature [7–10].

The Monte Carlo (MC) simulation of surface diffusion is one of the most reliable methods which can be used in order to study adparticle diffusion on different lattices and for various sets of the interaction parameters. However, the MC method is very time consuming and requires powerful computers.

In the present work we have investigated the diffusion of adsorbed particles on a square lattice by the RSRG approach. The results have been compared to corresponding MC data. We have explored and compared different physical situations, (1) repulsive and (2) attractive nearest neighbor (*nn*) interactions affecting the ground state of adsorbed particles, and two different diffusional

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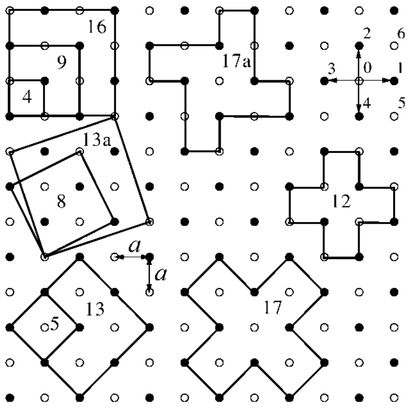

Fig. 1. $c(2\times 2)$ ordered lattice gas phase on a square lattice. Several blocks of sites used for RSRG transformations are shown. Arrows denote the four possible jumps of an adparticle.

mechanisms, which (a) consider and (b) neglect the interaction of the activated particle in the saddle point of the potential barrier with its nearest neighbors. Using a fully parallelized algorithm in conjunction with the Cray T3E (LC768-128) supermassive parallel computer operated by the Max-Planck community in Garching/Germany, we have investigated 11 different RSRG transformations with block sizes varying from 4 to 17 sites. We have explored the phase diagram of a square lattice gas with strong repulsion between the adparticles and the corresponding phase diagram of a 2D antiferromagnet in an external magnetic field. We have also calculated the coverage dependences of the chemical diffusion coefficient of adparticles for attractive and repulsive lateral interactions between adparticles. We have considered pairwise interactions of activated adparticles with their nearest neighbors and shown that these interaction changes drastically the behavior of the chemical diffusion coefficient.

The outline of this paper is as follows: the evolution equation and the expression for the diffusion coefficient are described in Section 2. The RSRG approach employed is discussed in Section 3 and details of the MC simulations are given in Section 4. The phase diagrams, adsorption isotherms and coverage dependences of different thermodynamic quantities and chemical diffusion coefficient are presented in Section 5.

2 Diffusion of particles on a square lattice

In the following we will consider an ideal solid surface of square symmetry. The potential relief minima of the surface form a two-dimensional square lattice with lattice constant a as shown in Figure 1. We will assume that adsorbed particles will occupy these lattice sites. If their adsorption energy ε is large relative to the thermal energy ($\varepsilon \gg k_{\mathrm{B}}T$) the adparticles will almost always be located in the minima, jumping from time to time to empty nn sites. In this case the thermodynamical state of the adparticle system is completely described by a set of site occupation numbers $\{n_i\}$ with

$$n_i = \begin{cases} 1 & \text{if the } i\text{th site is occupied,} \\ 0 & \text{if the } i\text{th is empty.} \end{cases} \tag{1}$$

Here the index $i = 1, 2, ..., N$ labels the N sites of the square lattice.

In thermodynamic equilibrium, the system is described by the statistical operator ρ,

$$\rho = Q^{-1} \exp \beta(\mu N_a - H_a) \tag{2}$$

with $\beta \equiv 1/k_{\mathrm{B}}T$. Here the number of adparticles N_a is given by

$$N_a = \sum_i n_i. \tag{3}$$

The system Hamiltonian H_a can be written as

$$H_a = -\varepsilon N_a + \varphi \sum_{\langle nn \rangle} n_i n_j \tag{4}$$

with μ as chemical potential, φ as pair interaction energy of particles adsorbed in the nn sites, symbol $\langle nn \rangle$ means that summation is performed over all lattice bonds just once.

The grand partition function Q appearing in equation (2) is written as

$$Q = \sum_{\{n_i\}} \exp \beta(\mu N_a - H_a). \tag{5}$$

The summation in equation (5) is carried out over all 2^N configurations of the adparticle system.

The occupation numbers change with time due to adparticle jumps. The balance equation for a given ith site can be written as

$$n_i(t + \Delta t) - n_i(t) = \sum_{nn} (J_{ji} - J_{ij}). \tag{6}$$

J_{ij} represents the number of jumps from the site i to the site j during the time interval Δt; the summation is carried out over four nns of the ith site. For small Δt one can define the regular and fluctuating parts of the particle flux as follows:

$$J_{ij} = (\nu_{ij} n_i h_j + \delta J_{ij}) \Delta t \tag{7}$$

where $h_j = 1 - n_j$, ν_{ij} is the frequency of jumps from the ith site to the jth site. The multiplier $n_i h_j$ ensures that the jump proceeds from occupied to empty sites only. The term $\delta J_{ij} \Delta t \equiv J_{ij} - \nu_{ij} n_i h_j \Delta t$ represents the jump fluctuations from the ith site to the jth site during the small time interval Δt.

Using equation (7) we can rewrite the balance equation (6) as

$$\frac{1}{\Delta t}[n_i(t + \Delta t) - n_i(t)] = \sum_{nn} (\nu_{ji} n_j h_i - \nu_{ij} n_i h_j) + \sum_{nn} (\delta J_{ji} - \delta J_{ij}). \tag{8}$$

The last sum on the RHS of equation (8) plays the role of the Langevin source of fluctuations $J_i^{\mathrm{L}}(t)$. Its correlation function was investigated in reference [11].

The balance equation (8) describes the relaxation kinetics of adparticle occupation numbers. The characteristic frequency of adparticle jumps is equal to $\langle \nu_{ij} n_i h_j \rangle$ (the angular brackets $\langle \cdots \rangle$ denote averaging with statistical operator ρ) and the characteristic length is equal to the lattice constant a. In general, the particle density fluctuations are large (any occupation number changes from 0 to 1 and *vice versa*), and it is impossible to solve the nonlinear balance equation or linearize it over small fluctuations of the occupation numbers. However, in many cases the detailed description of the relaxation is not required. If one considers the decay of the adparticle surface coverage fluctuations with characteristic length much larger than the lattice constant a, the decay of the coverage inhomogeneities proceeds as result of a great number of jumps of many adparticles and, therefore, the characteristic frequency must be much less than the mean frequency of adparticle jumps.

In the following we will consider states of the adparticle system averaged over a large time interval τ. The time interval τ must satisfy the inequality

$$\langle \nu_{ij} n_i h_j \rangle \tau \gg 1. \tag{9}$$

The averaging smears out all processes with characteristic frequencies $\omega \gtrsim \tau^{-1}$. During the time interval τ many adparticles visit any given site i. Thus, the fluctuations of the occupation numbers and other physical quantities, averaged over time τ, will be small because averages are taken over a large number of particles. It means also, that any site i comes into (quasi)equilibrium with its neighbors during the time interval τ. Any physically small region (its dimension must be about a) is described by a local-equilibrium statistical operator $\tilde{\rho}$ which has the form of the equilibrium operator ρ but contains the chemical potential of adparticles μ_i gradually varying in space and time. The averaged with the local-equilibrium operator physical quantities will also vary gradually in space and time. The relaxation of the quantities will describe by processes with characteristic space scales l and characteristic frequencies ω satisfying the following conditions

$$l \gg a \quad \text{and} \quad \omega \ll \tau^{-1}.$$

In order to obtain an explicit form of the local-equilibrium operator we develop the exponential term into a series of small deviations of the chemical potential $\delta\mu_i = \mu_i - \mu$ ($|\delta\mu_i/\mu| \ll 1$):

$$\tilde{\rho} = \tilde{Q}^{-1} \exp\Big[\beta\Big(\sum_i \mu_i n_i - H_a\Big)\Big] \approx \rho + \delta\rho = \rho\Big[1 + \beta \sum_i \delta\mu_i (n_i - \theta)\Big]. \tag{10}$$

Here $\theta \equiv \langle n_i \rangle$ is the mean surface coverage of adparticles.

The averaging of the balance equation with the local equilibrium statistical operator gives the following equation describing the evolution of the ith occupation number fluctuation,

$$\frac{\partial}{\partial t}\delta n_i(t) = \sum_{nn} [\delta(\nu_{ji} n_j h_i) - \delta(\nu_{ij} n_i h_j)] + J_i^{\mathrm{L}}(t) \tag{11}$$

with

$$\delta n_i = \beta \sum_j \delta\mu_j \langle n_i (n_j - \theta) \rangle,$$
$$\delta(\nu_{ij} n_i h_j) = \beta \sum_k \delta\mu_k \langle \nu_{ij} n_i h_j (n_k - \theta) \rangle. \tag{12}$$

It is justified to substitute the first relation in equations (12) by the following approximate expression

$$\delta n_i \approx \beta \delta\mu_i \sum_j (\langle n_i n_j \rangle - \theta^2) \equiv \frac{\partial \theta}{\partial \mu} \delta\mu_i, \tag{13}$$

which is valid if the correlation length ξ of the correlation function $\langle n_i n_j \rangle - \theta^2$ is small compared to the characteristic length of surface coverage fluctuations l. In order to obtain a closed equation for surface coverage fluctuations one must express adparticle flux fluctuations $\delta(\nu_{ij} n_i h_j)$ as explicit functions of adparticle surface coverage fluctuations δn_i. For this purpose one must know the mechanism of an adparticle jump. Here we restrict the considerations to nearest neighbor jumps. For example, an adparticle on site 0 can jump to one of its nearest neighbor sites 1, 2, 3 or 4 if the destination is empty as shown in Figure 1. The diffusing adparticle must surmount the potential barrier between the initial site and the final site. In case of interacting lattice gas the activation energies of jumps are affected by the presence of adjacent adparticles. Usually the interaction between an activated particle at the saddle point (SP) of the potential barrier and its nearest neighbors is neglected. Here we consider these interactions in the activated state by assuming that the adparticle in the saddle point interacts with its four *nn*s, labeled 2, 4, 5 and 6 in Figure 1. The corresponding interaction energy is given by φ_{sp} which, in the general case, is not equal to φ. Then, for the jump frequency ν_{01} one can write the following expression,

$$\nu_{01} = \nu \exp\{-\beta [\varepsilon + \varphi(n_2 + n_3 + n_4) - \varphi_{\mathrm{sp}}(n_2 + n_4 + n_5 + n_6)]\}. \tag{14}$$

Analogous expressions can be written easily for jump frequencies between other sites ν_{ij}. Inserting the expressions into equation (11) and developing slowly varying fluctuations of surface coverage into series up the first nonvanishing terms, one obtains, after some algebra, the ordinary diffusion equation with a diffusion coefficient determined by the following expression

$$D = D_0 P_{\mathrm{sp}} \exp(\beta\mu) \theta^{-1} \frac{\partial \beta\mu}{\partial \ln \theta}\,\cdot \tag{15}$$

Here $D_0 = \nu a^2 \exp(-\beta\varepsilon) \equiv D(\theta = 0)$ is the diffusion coefficient of noninteracting adparticles (Langmuir gas), $\partial\beta\mu/\partial \ln\theta$ is the thermodynamical factor and P_{sp} is the correlation factor

$$\begin{aligned} P_{\mathrm{sp}} = {} & \langle h_0 h_1 h_2 h_4 h_5 h_6 \rangle + 4A \langle h_0 h_1 n_2 h_4 h_5 h_6 \rangle \\ & + 2A^2 \big(\langle h_0 h_1 n_2 n_4 h_5 h_6 \rangle + \langle h_0 h_1 n_2 h_4 h_5 n_6 \rangle \\ & + \langle h_0 h_1 n_2 h_4 n_5 h_6 \rangle\big) + 4A^3 \langle h_0 h_1 n_2 n_4 n_5 h_6 \rangle \\ & + A^4 \langle h_0 h_1 n_2 n_4 n_5 n_6 \rangle. \end{aligned} \tag{16}$$

Here we used the abbreviation $A = \exp(-\beta\varphi_{\rm sp})$.

It should be noted that for $\varphi_{\rm sp} = 0$, *i.e.* neglecting the interactions of particles in the activated state, the correlation factor reduces to a rather simple expression, $P_{00} \equiv \langle h_0 h_1\rangle$ (the correlation function of two *nn* holes). Due to its simplicity, this approximation is used widely in many papers concerned with surface diffusion.

Introducing the free energy of the system F as

$$F = k_{\rm B}TN^{-1}\ln Q, \tag{17}$$

it is possible to calculate all quantities in equation (15) *via* the following first and second derivatives of the free energy:

$$\theta = \frac{\partial F}{\partial \mu}, \tag{18}$$

$$\begin{aligned} P_{00} &= \langle(1-n_i)(1-n_1)\rangle \\ &= 1 - 2\theta + \langle n_i n_1\rangle = -\frac{1}{2}\frac{\partial F}{\partial \varphi}, \end{aligned} \tag{19}$$

$$\frac{\partial \mu}{\partial \ln\theta} = \theta\left(\frac{\partial^2 F}{\partial \mu^2}\right)^{-1}. \tag{20}$$

The correlation functions of higher orders can be calculated as the first derivatives of the free energy over some fictious multiparticle interaction parameters, which correspond to the respective adparticle configurations. These first derivatives are smooth functions of chemical potential and surface coverage and do not exhibit singular behavior at the critical points. Therefore, simple approximations can be used to estimate the correlation functions. For instance, one can approximate 6-sites correlation functions as a product of three nearest neighbor pair sites correlation functions,

$$\begin{aligned}
\langle h_0h_1h_2h_6h_4h_5\rangle &\approx \langle h_0h_1\rangle\langle h_2h_6\rangle\langle h_4h_5\rangle = P_{00}^3\\
\langle h_0h_1n_2h_6h_4h_5\rangle &\approx \langle h_0h_1\rangle^2\langle n_0h_1\rangle = (1-\theta-P_{00})P_{00}^2\\
\langle h_0h_1n_2n_6h_4h_5\rangle &\approx \langle h_0h_1\rangle^2\langle n_0n_1\rangle = (2\theta-1+P_{00})P_{00}^2\\
\langle h_0h_1n_2h_6n_4h_5\rangle &\approx \langle h_0h_1\rangle\langle n_0h_1\rangle^2 = (1-\theta-P_{00})^2P_{00}\\
\langle h_0h_1n_2n_6n_4h_5\rangle &\approx \langle h_0h_1\rangle\langle n_0n_1\rangle\langle n_1h_1\rangle = (1-\theta-P_{00})\\
&\qquad\times(2\theta-1+P_{00})P_{00}\\
\langle h_0h_1n_2n_6n_4n_5\rangle &\approx \langle h_0h_1\rangle\langle n_0n_1\rangle^2 = (2\theta-1+P_{00})^2P_{00}.
\end{aligned} \tag{21}$$

Using these approximations, one can reduce equation (16) to

$$P_{\rm sp} = P_{00}\left[P_{00} + 2A(1-\theta-P_{00}) + A^2(2\theta-1+P_{00})\right]^2. \tag{22}$$

The only quantity one must know is the free energy F for the system of adparticles. However, it is important to recall that this is a reasonable assumption only in the hydrodynamic limit (*i.e.* for adparticle surface coverage inhomogeneities varying slowly in space and time and only if the adparticle jump frequency is determined by Eq. (14)).

3 Real-space renormalization group transformations on square lattice

For the determination of the free energy of the system F approximate methods are required. Even for the simplest model with *nn* interactions, the problem remains too complex to be solved exactly. The well-known Onsager solution [12] for 2D Ising spin model was obtained in zero magnetic field, which is equivalent to half monolayer surface coverage ($\theta = 0.5$).

In this section we will briefly outline the RSRG method used for this purpose. It is well-known that the lattice gas model is equivalent to the Ising spin model in an external magnetic field. Empty sites are equivalent to $s = -1$, and occupied sites to $s = 1$. Using the obvious relation between site spins and occupation numbers

$$n_i = (1 + s_i)/2, \tag{23}$$

one can obtain easily the equivalent reduced Hamiltonian of the Ising model in the following form

$$-\beta H(s) = h\sum_i^N s_i + k\sum_{\langle nn\rangle} s_is_j + Nc. \tag{24}$$

Here $h = \beta(\mu+\varepsilon-2\varphi)/2$, $k = -\beta\varphi/4$, $c = \beta(\mu+\varepsilon-\varphi)/2$.

As the chemical potential of adparticles is equivalent to the external magnetic field, there is a one to one correspondence between thermodynamic properties of the lattice gas and magnetic properties of the Ising spin system. Although the lattice gas model (Eq. (4)) and Ising spin model (Eq. (24)) are fully equivalent, we prefer to use the spin representation in the following because of its symmetry with respect to the magnetic field. However, we will refer to lattice gas terms where this seems to be more transparent.

Strong lateral interactions cause phase transitions. In the present work we consider ferromagnetic (F) and antiferromagnetic (AF) interactions between the spins (in lattice gas terminology these interactions represent attraction or repulsion between adjacent adparticles). The exact critical value of the interaction parameter k^* is equal to $0.5\ln(1+\sqrt{2}) \approx 0.440\,686\,79$ [13].

In the RSRG method developed by Niemeyer and van Leeuwen [14] and Nauenberg and Nienhuis [15,16], the whole lattice is divided into blocks (or cells) of L sites [17]. A block spin S_α is assigned to each block. All blocks together must form a square lattice with the lattice constant $\sqrt{L}a$. The RSRG transformation of the spin system allows the reduction of the number of independent variables, *i.e.* the transition from the set of N site spins $\{s_i\}$ to N/L block spins $\{S_\alpha\}$. The transformation can be described by

$$\exp[H(S) + g] = \sum_{\{s\}} P(S,s)\exp[H(s)], \tag{25}$$

where $H(S)$ is the renormalized Hamiltonian of the block spin system, g is the self-energy per spin of the block, which plays an important role in the RSRG method. $P(S,s)$ is the weighting factor given by

$$P(S,s) \geq 0 \quad \text{and} \quad \sum_{\{S\}} P(S,s) = 1. \tag{26}$$

We note that two values of the block spin $S_\alpha = \pm 1$ corresponds to 2^L site spin configurations (since L spins are combined to form a block). Using the weighting factor one can distribute the configurations into the domains, corresponding to definite values of the block spin. For blocks with odd number of spins S_α is usually determined by the so-called "majority rule" (MR) [18]

$$S_\alpha = \operatorname{sgn}\left(\sum_{i=1}^{\mathrm{L}} s_i\right) \tag{27}$$

with

$$\operatorname{sgn}(x) = \begin{cases} +1, & \text{if } x > 0, \\ -1, & \text{if } x < 0. \end{cases} \tag{28}$$

For this case the weighting factor can be written as

$$P(\{S_\alpha\},\{s_i\}) = \prod_\alpha \frac{1}{2}\left[1 + S_\alpha \operatorname{sgn}\left(\sum_{i=1}^{\mathrm{L}} s_i\right)\right]. \tag{29}$$

The weighting factor assigns weights 1 or 0 to the site spin configurations depending on the sign of the sum of all site spins entering the block. Of course, the choice of equation (29) for the weighting factor is not unique. For even L a rule must be introduced in order to assign a definite value of the block spin to any given configuration with the sum of site spins equal to zero. In any case an obvious condition must be fulfilled: if the site spin configuration $\{s_1, s_2 \ldots s_L\}$ is assigned to a block spin S_α with weighting factor P, then the configuration $\{-s_1, -s_2 \ldots - s_L\}$ is assigned to the $-S_\alpha$ domain with the same P.

The main idea of the RSRG transformation is that the result of the summation would have the same form as the original Hamiltonian (Eq. (24)) plus insignificant terms, which weakly affect the critical behavior of the system. In order to carry out the summation in equation (25) some approximations must be used. In the framework of the RSRG approach, one usually employs periodic boundary conditions. It is assumed that the whole lattice is given by the periodic continuation of a small cluster of blocks. In the present work we consider the smallest possible cluster of two blocks. Due to the simplicity of this cluster, no additional interactions appear in the renormalized Hamiltonian. It is the same Hamiltonian of the square Ising spin system with, however, renormalized values for the external magnetic field h_1 and for the *nn* pair interaction parameter k_1. The relations between renormalized and original values of the interaction parameters of equation (24) are given by

$$h_1(S_1+S_2) + 4k_1 S_1 S_2 + g = \ln\left\{\sum_{\{s\}} P(S,s)\exp[H(s)]\right\} = \Psi(S_1,S_2). \tag{30}$$

Here the summation is carried out over all possible configurations $\{s_i\}$ for fixed values of the block spins $S_{1,2}$. The solution of the equation is the system of renormalization equations

$$\begin{aligned} h_1 &= (\Psi_{++} - \Psi_{--})/4 \\ k_1 &= (\Psi_{++} + \Psi_{--} - 2\Psi_{+-})/16 \\ g &= (\Psi_{++} + \Psi_{--} + 2\Psi_{+-})/2L. \end{aligned} \tag{31}$$

Here $\Psi_{\pm\pm} \equiv \Psi(S_1,S_2)$ represents the RHS of equation (30) with definite values of the block spins S_1 and S_2. The functions $\Psi_{\pm\pm}$ have the following properties due to the symmetry of the Hamiltonian (Eq. (24)),

$$\begin{aligned} \Psi_{+-}(h,k) &= \Psi_{-+}(h,k), \\ \Psi_{--}(h,k) &= \Psi_{++}(-h,k). \end{aligned}$$

The most important property of any RSRG transformation is the existence of fixed points of the system equations (31), where the transformation is analytic. The fixed points are determined by the conditions $h_1 = h$ and $k_1 = k$. The nontrivial (*i.e.*, not $h = k = 0$) unstable fixed points of the system correspond to the critical points of the Hamiltonian (Eq. (24)). From the symmetry of the first equation of equation (31) it is obvious that all fixed points are located on the k-axis ($h_\mathrm{c} = 0$). In order to determine the stability of the fixed point $(h_\mathrm{c}, k_\mathrm{c})$, one must investigate the properties of the transformation at this point. In the vicinity of any fixed point one can linearize the RSRG transformation

$$\begin{aligned} h_1 - h_\mathrm{c} &= T_{hh}(h - h_\mathrm{c}) + T_{hk}(k - k_\mathrm{c}), \\ k_1 - k_\mathrm{c} &= T_{kh}(h - h_\mathrm{c}) + T_{kk}(k - k_\mathrm{c}). \end{aligned} \tag{32}$$

The matrix

$$\hat{T} = \begin{pmatrix} \dfrac{\partial h_1}{\partial h} & \dfrac{\partial h_1}{\partial k} \\ \dfrac{\partial k_1}{\partial h} & \dfrac{\partial k_1}{\partial k} \end{pmatrix}$$

describes the linear response of the renormalized parameters of the Hamiltonian (Eq. (24)), h_1 and k_1, on variations of the original values h and k around the fixed points. This matrix has two eigenvalues: λ_h and λ_k. The condition for critical behavior is the existence of eigenvalues $\lambda_{h,k} > 1$ (unstable fixed points). The eigenvalues are related to the critical exponents of the 2D Ising model α (describes power behavior of the specific heat) and δ (describes response to an external magnetic field at critical temperature T_c) *via* [19]:

$$\alpha = 2 - \frac{\ln L}{\ln \lambda_k}, \tag{33}$$

and

$$\delta = \frac{\ln \lambda_h}{\ln L - \ln \lambda_h} \cdot \tag{34}$$

It is well-known that for the 2D Ising spin model the exact values of these critical indices are $\alpha = 0$ and $\delta = 15$.

Table 1. Critical values of interaction parameters and critical indices α and δ for attractive (F) and repulsive (AF) pair interactions. The first column shows the number of the block in Figure 1.

#	cluster	k_c (F)	ϵ (%)	α (F)	δ (F)	$\lvert k_c \rvert$ (AF)	ϵ (%)	α (AF)	δ (AF)
4	4×2	0.5287	20	−0.75	33.7	a			
5	5×2	0.4822	9.4	−0.60	21.4	0.4822	9.4	−0.65	0.21
8	8×2	0.4588	4.1	−0.56	16.8	a			
9	9×2	0.4533	2.9	−0.41	16.6	a			
12	12×2	0.5088	15.5	−0.64	32.8	a			
13	13×2	0.4533	2.85	−0.41	16.8	0.4694	6.5	−0.48	0.30
13a	13×2	0.4476	1.56	−0.43	15.4	0.5860	33	−1.36	0.23
16	16×2	0.4485	1.78	−0.34	16.1	a			
17	17×2	0.44011	0.13	−0.38	14.4	0.44414	0.8	−0.38	0.33
17	$17 \times 2^*$	0.44414	0.8	−0.38	14.3	0.44011	0.13	−0.38	−0.3
17a	17×2	0.44540	1.0	−0.35	15.3	a			

* Critical data are obtained with AF MR. ^{a}AF critical point is absent.

Therefore, the exact RSRG transformation should have two nontrivial fixed points $(0, \pm k^*)$ with $\lambda_k^* = \sqrt{L}$ and $\lambda_h^* = L^{15/16}$. Comparing the computed values of k_c, λ_h and λ_k with the exact ones, gives a valuable measure for the precision of the RSRG transformation.

As was shown by Nauenberg and Nienhuis [15], the free energy of the system for any values of magnetic field and interaction parameter $F(h,k)$ can be evaluated in the series of sequential RSRG transformations of the original Hamiltonian (Eq. (24))

$$F(h,k) = k_B T \sum_{m=0}^{n} L^{-m} g(h_m, k_m) + F(h_n, k_n) L^{-n}. \tag{35}$$

Here h_m and k_m are the parameters of the mth RSRG transformation, $h_0 = h$, $k_0 = k$.

In the limit $n \to \infty$ the last term in the RHS of equation (35) tends to zero. It should be noted, that for large L infinite-series solution converges very fast for all values of parameters h and k.

We have investigated 11 RSRG transformations with 10 different blocks, shown in Figure 1. We have considered finite lattices consisting of a cluster with periodic boundary conditions and every cluster consists of $2L$ different site spins or 2 block spins. The transformations are denoted as $L \times 2$.

All RSRG transformations have some general properties. Usually, RSRG transformations with odd L have two fixed points; one in the ferromagnetic (F) region ($k_c > 0$) and another one in the antiferromagnetic (AF) one ($k_c < 0$). For even L all RSRG transformations have only one fixed point in the F region. In general, the critical values of the interaction parameter k_c approach the exact value k^* if the number of spins in the block is increased. However, the accuracy of a transformation depends considerably not only on the block size L, but also on the symmetry of the block. It seems that the symmetry plays decisive role. The most symmetrical blocks have the best properties. This is clearly seen if one compares results obtained for RSRG transformations with the same L but with different symmetry of the blocks, $L = 13$ and 17 (see Tab. 1). Less symmetrical blocks give worse results.

The most accurate results are obtained for RSRG transformation with two symmetrical blocks of 17 spins each (cluster 17×2) with relative errors in determining the critical value of pair interaction parameter $\epsilon \equiv (|k_c - k^*|/k^*)100\% \simeq 0.13\%$.

In the present work we have used also antiferromagnetic majority rule (AFMR), which can be written in the form of equation (27), but spins from different sublattices appear in the sum with different signs. The ordinary MR selects configurations depending on their ferromagnetic ordering (total magnetic moment of the block), but the AFMR prefers AF ordered configurations (difference of the magnetic moments of sublattices). The results are rather simple. Using AFMR we have obtained the same absolute values of the critical points but they change their signs. F critical point became AF critical point and *vice versa.*

In Table 1 the critical values are compiled for the different clusters studied in the present work. The critical values for the $17 \times 2^*$ RSRG transformation have been obtained using the AFMR.

4 The Monte Carlo simulation of surface diffusion

The Monte Carlo technique is one of the most universal methods which is used widely to study complex phenomena especially when analytical approaches are not available or work badly. For a detailed description of the application of the MC approach to the investigation of surface diffusion the interested reader is reffered to reference [20]. In our MC algorithm, the system with the Hamiltonian given by equation (24) is realized by a 2D array of $N \times N$ sites with periodic boundary conditions. The saddle point energies (describing the wells which need to be overcome by adparticles) are uniformly given by a common value, ε, throughout the whole lattice. It is assumed that the saddle point energies are not affected by adparticle-adparticle interactions.

Initial lattice gas configuration are generated by throwing θN^2 particles at random on the surface. The jump algorithm can be summarized as follows: first, an initial site i of the whole lattice is picked at random, if filled, an adjacent final site j is randomly selected. If this destination is vacant, a jump can occur with a probability given by $P_{ij} \propto \exp(-E_{ij}/k_{\mathrm{B}}T)$. E_{ij} denotes the activation energy for this jump and can be calculated as the energy difference between saddle point and the energy of the initial site ε_i, the latter being influenced by nearest neighbor interactions as already mentioned, $E_{ij} = \varepsilon - \varphi \sum_{nn} n_j$. One MC step (MCS) corresponds to N^2 interrogations of lattice sites in random order. A large number of initial MCS's were performed before any quantity is calculated in order to establish a desired temperature T and to reach thermodynamic equilibrium. As in reference [21], the approach to equilibrium is monitored by following the total energy and is assumed to occur when this quantity fluctuates about an average value. The time (in units of MCS's) needed for equilibration depends on the lattice size, temperature and coverage. Typically, 2×10^4 MCS are required to establish equilibrium in lattices containing up to 64×64 sites. In order to obtain accurate values of the different quantities, runs of up to 8×10^4 for up to 256 different initial configurations were performed.

The chemical diffusion coefficient D has been determined *via* the fluctuation method, which measures the particle number autocorrelation function $f_n(t)/f_n(0)$ for a small probe region embedded in the whole lattice. The autocorrelation function can be written as

$$f_n(t)/f_n(0) = \frac{\langle \delta N_p(t) \delta N_p(0) \rangle}{\langle \delta N_p^2 \rangle}\,. \tag{36}$$

Here, N_p is the number of adparticles in the probe area. Details of this methods are presented in references [22,23]. The ratio $f_n(t)/f_n(0)$ is then compared with the theoretical curve, yielding value of the diffusion coefficient [24]. Thus, this method is a computer simulation of the field emission fluctuation method used experimentally to determine chemical diffusion coefficient.

The thermodynamic factor is obtained in either one of its two equivalent forms

$$\left(\frac{\partial \beta \mu}{\partial \ln \theta}\right) = \left[\frac{\langle (\delta N)^2 \rangle}{\langle N \rangle}\right]^{-1} \tag{37}$$

either *via* the differentiation of adsorption isotherms or *via* the normalized mean square fluctuations equation (37).

5 Results and discussion

For calculations we have used the most accurate 17×2 RSRG transformation with MR for attractive pair interaction and AFMR for repulsive lateral interaction.

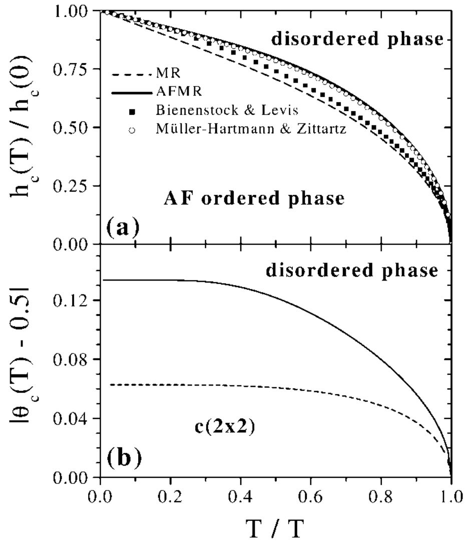

Fig. 2. Phase diagram for (a) antiferromagnetic Ising spin system on a square lattice and (b) lattice gas with lateral repulsion between adparticles on a square lattice. The solid lines are obtained with the antiferromagnetic majority rule (AFMR) and the dashed curves represent the ordinary majority rule (MR). The squares are calculated according to Bienenstock and Levis [26] and the circles represent the data obtained by reference [27].

We have calculated the phase diagram for the two-dimensional spin antiferromagnet (and the corresponding lattice gas with repulsive nearest neighbor interactions) using the ordinary MR and AFMR. The positive h part of the critical line is shown in Figure 2a. The critical temperature can be represented by the following simple expressions [25]

$$T_{\mathrm{c}}(h) = \begin{cases} T_{\mathrm{c}}(0)[1 - (h/h_{\mathrm{c}})^2], & \text{for MR} \\ T_{\mathrm{c}}(0)[1 - (h/h_{\mathrm{c}})^{2.31}]^{0.8}, & \text{for AFMR.} \end{cases} \tag{38}$$

Here $h_{\mathrm{c}} = 4|k|$ is the critical magnetic field at zero temperature, $T_{\mathrm{c}}(0) = 0.56818\varphi/k_{\mathrm{B}}$.

The critical values of the external magnetic field are determined by the coordination number of lattice z: $h_{\mathrm{c}} = \pm zk$ (for square lattice $z = 4$). All RSRG transformations yield the exact values for h_{c}.

Bienenstock and Levis presented a slightly different functional dependence for the critical temperature,

$$T_{\mathrm{c}}(h) = T_{\mathrm{c}}(0)[1 - (h/h_{\mathrm{c}})^2]^{0.87}. \tag{39}$$

This expression was obtained using high-temperature expansions of the free energy [26]. The corresponding critical line is also shown in Figure 2a and is located just between the critical lines given by our MR/AFMR expressions (Eq. (38)). It should be noted that the critical line obtained by the AFMR is in very good agreement with the simple expression supposed by Müller-Hartmann and Zittartz [27],

$$\cosh(h_{\mathrm{c}}) = \sinh^2(2k_{\mathrm{c}}), \tag{40}$$

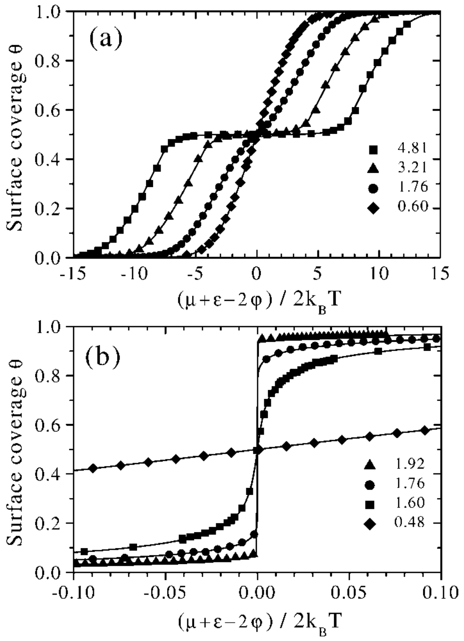

Fig. 3. Adsorption isotherms (surface coverage θ *versus* the normalized chemical potential $\mu/k_{\mathrm{B}}T$ for several values of the reciprocal temperature expressed in units of $|\varphi|/k_{\mathrm{B}}T$ and for (a) repulsive and (b) attractive interactions between adatoms. Solid lines are obtained by the RSRG method, symbols denote MC data.

which is also shown in Figure 2a. The deviations between the critical lines obtained by the MR and AFMR RSRG approaches are relatively small in the h–T representation of the phase diagram, but much stronger deviations arise when we consider the phase boundary between ordered and disordered lattice-gas phases in the θ–T representation (see Fig. 2b). The ordinary MR approach yields a very narrow region near half coverage for the existence of the ordered phase, $0.437 \lesssim \theta \lesssim 0.563$ (dotted curve in Fig. 2b). The AFMR approach gives a significantly wider stability range of this phase, $0.363 \lesssim \theta \lesssim 0.637$ (full curve in Fig. 2b). This range coincides rather well with the results obtained by Runnels and Combs [28], $0.371 \lesssim \theta \lesssim 0.629$.

Adsorption isotherms $\theta(\mu)$ for repulsive and attractive interactions between adparticles are shown in Figures 3a and 3b, respectively. The RSRG results are shown as solid lines. The coincidence between RSRG and MC data (symbols in Fig. 3) is obviously very good for all temperatures and for all surface coverages studied. At high temperatures the dependences are close to the Langmuir case ($\varphi = 0$)

$$\theta(\mu) = \exp(\mu + \varepsilon)\,[1 + \exp(\mu + \varepsilon)]^{-1}\,. \tag{41}$$

As the temperature decreases the behavior of the curves becomes quite different. For antiferromagnetic/repulsive interactions a peculiarity appears at half coverage which turns into a broad almost horizontal plateau at temperatures well below T_{c}. The plateau represents the formation of the ordered $c(2 \times 2)$ phase, shown in Figure 1. For ferromagnetic/attractive interactions the adsorption isotherms exhibit jumps of the surface coverage θ (or magnetization $m = \langle s_i \rangle$), which corresponds to the first order phase transition between two lattice gas phases with different surface coverages.

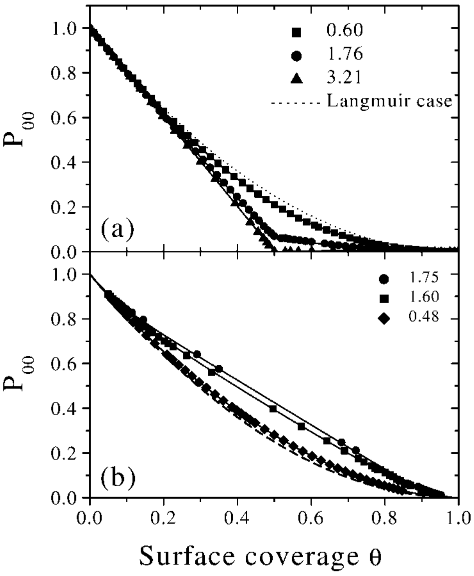

Fig. 4. Surface coverage dependence of the pair correlation function P_{00} for (a) repulsive and (b) attractive interactions between adatoms. The curves are labeled according to their temperatures expressed in units of $|\varphi|/k_{\mathrm{B}}T$. Solid lines are obtained by the RSRG approach, symbols denote MC data. The dashed lines represent the mean-field result $P_{00} = (1-\theta)^2$.

We have also investigated the coverage dependence of the correlation function P_{00}, which is needed to calculate the chemical diffusion coefficient D. For repulsive and attractive interactions as well, P_{00} is a smooth function of the surface coverage (see Figs. 4a and 4b, respectively). At high temperatures P_{00} is close to the mean-field result $P_{00} = (1-\theta)^2$. For repulsive interaction and low temperatures P_{00} decreases almost linearly to very small values at half coverage, *i.e.* $P_{00} \approx 1 - 2\theta$ for $0 < \theta < 1/2$ (Fig. 4a). This result is clearly due to the fact that at these coverages adparticles are able to avoid each other and, therefore, every particle adsorbing on the surface destroys 4 two-hole configurations. Thus, the probability to find such configurations can be expressed as $1 - 4 \times$ (number of particles)/(number of bonds) $= 1 - 2\theta$. In contrast, attractive interactions increases the probability of finding pairs of *nn* adparticles and, therefore, the number of *nn* holes increases also. Again, the coincidence between RSRG (lines) and MC data (symbols) is rather good throughout the whole range of temperatures and coverages.

The quantity which is the most sensitive to the phase transition is the isothermal susceptibility χ_T. This quantity is defined as the mean square fluctuations of the magnetization of the spin system, which corresponds to the mean square surface coverage fluctuations in lattice gas systems

$$\chi_T = \frac{1}{k_{\mathrm{B}}T}\left(\frac{\partial^2 F}{\partial h^2}\right)_T = \langle s_i s_j \rangle - m^2 \equiv 4\langle n_i n_j \rangle - \theta^2 \tag{42}$$

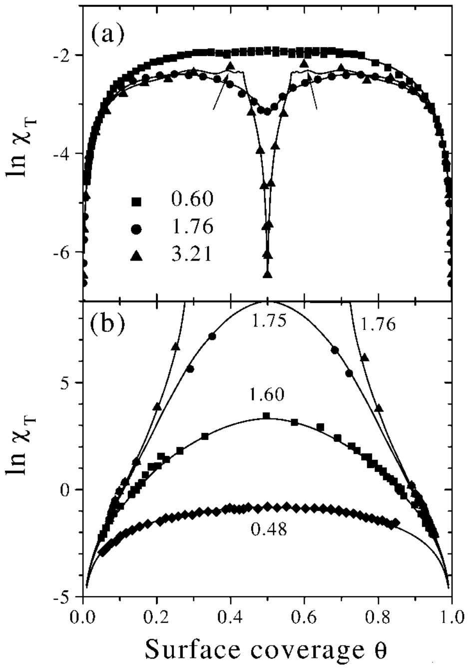

Fig. 5. Coverage dependence of the isothermal susceptibility in case of (a) repulsive and (b) attractive interactions between adatoms. The curves are labeled according to their temperatures expressed in units of $|\varphi|/k_{\mathrm{B}}T$. Solid lines are obtained by the RSRG approach, symbols denote MC data.

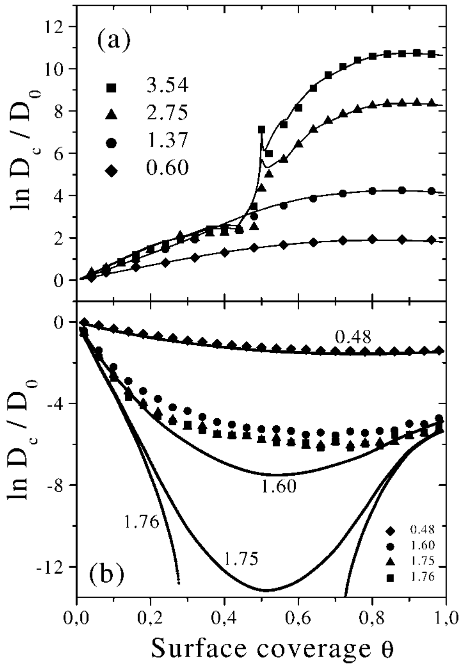

Fig. 6. Coverage dependence of the chemical diffusion coefficient in case of (a) repulsive and (b) attractive interactions between adatoms. The curves are labeled according to their temperatures expressed in units of $|\varphi|/k_{\mathrm{B}}T$. Solid lines are obtained by the RSRG approach, symbols denote MC data.

The coverage dependence of this quantity is shown in Figures 5a and 5b for the cases of repulsive and attractive energy interactions between adsorbed particles, respectively. At high temperatures (Langmuir case) the mean square surface coverage fluctuations are equal to $\theta(1-\theta)$. In case of repulsive interactions (Fig. 5a) there are deep and narrow minima at half coverage and low temperatures. These conditions correspond to an almost perfectly ordered $c(2\times 2)$ structure. Under these conditions any coverage disturbance (*i.e.*, the displacement of an adparticle from its "right" position in the filled sublattice to any site of the empty sublattice) increases considerably the energy of the system and is thermodynamically unfavorably. Thus mean square coverage fluctuations are suppressed. For coverages $\theta \neq 0.5$, there are fluctuations of nonstoichiometric nature that do not require additional energy for their existence. These fluctuations cannot by removed from the system by adparticle jumps. Therefore, χ_T increases when θ deviates from half coverage. It is also interesting to note that at low temperatures the fluctuations have tiny maxima on the critical line $T_{\mathrm{c}}(\theta)$ (see the arrows in Fig. 5a). The behavior is nonanalytical in these points. It should be noted that the most pronounced deviations between RSRG and MC data arise in the vicinities of these points.

For attractive interactions the mean square surface coverage fluctuations are strongly divergent in the critical point. The critical behaviour is well described by a power law, obtained by the RSRG approach as

$$\chi_T \propto (T - T_{\mathrm{c}})^{\gamma} \tag{43}$$

with

$$\gamma = (2-\alpha)\frac{\delta-1}{\delta+1} \approx 2.06. \tag{44}$$

The exact value of the critical index for the Ising spin model is well-known as $\gamma = 7/4$.

Isothermal coverage dependences of the chemical diffusion coefficient are shown in Figures 6a and 6b for repulsive and attractive energy interactions between adsorbed particles, respectively. We consider first the case $\varphi_{\mathrm{sp}} = 0$. In the limits of $\theta \to 0, 1$, a jumping adparticle has none or three nearest neighbors, respectively. Therefore, the limiting values of the diffusion coefficient are equal to

$$\begin{aligned} &\lim_{\theta\to 0} D = D_0, \\ &\lim_{\theta\to 1} D = D_0 \exp\left(-3\beta\varphi\right). \end{aligned} \tag{45}$$

We will first discuss the case of repulsive nearest neighbor interactions (Fig. 6a). For small surface coverages $\theta \ll 0.5$, *i.e.* in the disordered lattice gas phase, $\ln D$ changes almost linearly with θ. This behavior reflects the increase of the mean number of nearest neighbors for any jumping adatom. It is interesting to note that qualitatively similar behavior can be seen at large coverages slightly below full coverage, where $\ln D$ decreases almost linearly with θ. In this case the relaxation of coverage fluctuations proceeds *via* the diffusion of holes, whose concentration is given by $\theta_h = 1-\theta$. Therefore, the linear decrease of $\ln D$ with θ is comprehensible. It is probably important to note, that due to the particle-hole symmetry of the lattice gas Hamiltonian, the repulsive interaction energy for holes is also given by φ. In the vicinity of half coverage the $c(2 \times 2)$ lattice gas phase is stable. There are two peculiarities of the diffusion coefficient associated with this ordered phase, (i) a strong and sharp maximum at $\theta = 0.5$, *i.e.* when the ordering is best, and (ii) two tiny minima at the critical lines corresponding to the second order phase transition between dilute lattice gas ↔ $c(2 \times 2)$phase ↔ dense lattice fluid. Upon approaching the critical lines, the density fluctuations grow and cause the reduction of the diffusion coefficient. The minima of the diffusion coefficient corresponds to maxima of the mean square surface coverage fluctuations, see Figure 5a.

Attractive interaction between *nn*s reduces mobility of adparticles. The chemical diffusion coefficient decreases relative to the Langmuir case: $D(\theta) < D_0$ for all surface coverages and $\ln D$ exhibits a broad minimum at coverages around $\theta \approx 0.5$ (Fig. 6b). The RSRG results predict dramatic changes of the diffusion coefficient, if the temperature approaches T_c (where the attractive interaction causes the first order phase transition). The chemical diffusion coefficient tends to zero at the critical points. We conclude that the critical slowdown of the chemical diffusion coefficient in essence is described by the critical behavior of the isothermal susceptibility χ_T (Eq. (43)). This conclusion is based on the fact, that all other quantities entering equation (15) vary slowly in the critical region [6].

In the following paragraphs we will discuss the influence of saddle point interactions on the chemical diffusion coefficient. In Figure 7 we show the isotherms of the coverage dependence of this quantity for repulsive (Fig. 7a) and attractive (Fig. 7b) *nn* interaction φ. The various curves are labelled according to the corresponding ratio $\varphi_\mathrm{sp}/\varphi$. In all cases we assume that the attractive/repulsive character of the interactions in the ground state and activated state is maintained. Figure 7a clearly indicates that repulsive interactions in the activated state generally reduce the chemical diffusion coefficient (relative to the case $\varphi_\mathrm{sp} = 0$). In order to explain this finding we recall that repulsive interactions in the activated state raise the effective barrier height of the corresponding jump event. Thus the jump probabilities are reduced and the diffusion is slowed down. The effect of attractive saddle point interactions (Fig. 7b) is just the opposite. Lowering the effective barrier height for nearest neighbor jumps result in an overall increase of the chemical diffusion coefficient. If we consider that a jumping adatom may have up to three nearest neighbors in the ground state and up to four nearest neighbors in the saddle point, we can approximate the limiting value of the chemical diffusion coefficient for $\theta \to 1$ as

$$\lim_{\theta \to 1} D = D_0 \exp\left[\beta(4\varphi_\mathrm{sp} - 3\varphi)\right]. \qquad (46)$$

Figures 7a and 7b indicate that the changes induced by saddle point interactions are relatively small (*i.e.* the general shape of the curves are maintained) if the saddle point interactions are a small fraction of the interaction energy, $\varphi_\mathrm{sp}/\varphi < 1$. However, if both quantities become comparable or if φ_sp numerically exceeds φ, then the situation may arise that repulsive interactions reduce and attractive interactions enhance chemical diffusion relative to the Langmuir case. However, even then the peculiarities of the chemical diffusion coefficient related to the formation of the $c(2\times2)$ lattice gas phase (Fig. 7a), *i.e.* the maximum of D at $\theta = 0.5$ and the two minima at the critical coverages θ_c), are clearly visible (albeit less pronounced).

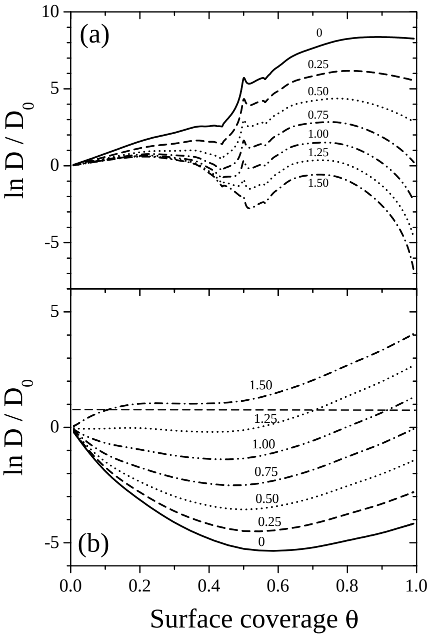

Fig. 7. Coverage dependence of the chemical diffusion coefficient in case of (a) repulsive and (b) attractive interactions between adatoms for a temperature given by $|\varphi|/k_\mathrm{B}T = 2.75$ and $|\varphi|/k_\mathrm{B}T = 1.37$, respectively. The curves are labeled according to the ratio $|\varphi_\mathrm{sp}|/|\varphi|$. All lines are obtained by the RSRG approach.

6 Summary

We have investigated 11 RSRG transformations on the square lattice with 10 blocks of different symmetries with sizes varying from 4 to 17 sites per block. It has been shown that the precision of the method depends strongly not only on the number of sites in the block but also on its symmetry. In general, the accuracy of the method increases with the number of sites in the block. The most accurate results have been obtained for the biggest cluster 17×2. The minimal relative error in determining the critical value of the interaction parameter is equal to 0.13%. It has been shown that using of the antiferromagnetic majority rule gives significantly better results for the repulsive interactions between adparticles as compared to the ordinary majority rule.

One should expect, of course, that errors must tend to zero when block size L goes to infinity. But even rather small clusters 9×2, 13×2 have very good characteristics and can be used successfully for investigations of the thermodynamic properties of the Ising spin and lattice gas systems. And 17×2 RSRG transformations has extremely good accuracy comparable with accuracy of the best MC simulations.

It should be noted that different critical parameters of RSRG transformations converge to its exact values with different speeds when block size L is increased. For example, the critical magnetic field h_c at zero temperature has its exact value for all RSRG transformations independently on the block size, the critical values of the interaction parameter k_c for F and AF interactions have rather good tendencies of convergence to their exact values. It is seen from the Table 1 that the critical indices α and δ have different behaviors when L is increased from 4 to 17. The values of critical indices are determined by the eigenvalues $\lambda_{h,k}$ of the linear response matrix $\hat{T}$ for a given RSRG transformation. Critical index α (determined entirely by λ_k) tends slowly to $\alpha^* = 0$, but another critical index δ (determined by λ_h) converges rapidly to its exact value $\delta^* = 15$.

Also, necessary to note that the values of the critical index δ differ considerably for the F and AF interactions. It follows from the properties of the RSRG transformations that the isothermal susceptibility of the Ising antiferromagnet has not power divergence at the critical point. It is connected with the quite different behavior of the Ising spin systems with F and AF pair interactions in the external magnetic field. The ferromagnetic susceptibility has strong power divergence. For a ferromagnet Ising system all correlations add to give a large critical index $\gamma = 7/4$. The RSRG approach gives $\gamma = 2.06$. This value corresponds to qualitatively right power law critical dependence of the isothermal susceptibility. For an antiferromagnet the correlations cancel each other and the residual divergence is much weaker. The temperature series gives logarithmic divergence of the antiferromagnetic susceptibility at the critical point similar to the critical behavior of the super-exchange model, derived by Fisher [29] (see also review article Ref. [30]). The logarithmic divergence of the isothermal susceptibility at the AF critical point corresponds to $\gamma_{\mathrm{AF}} = 0$ or $\delta_{\mathrm{AF}} = 1$. The values of δ_{AF} in the last column of the Table 1 are substantially deviated from this value. The negative values of the critical index $-1 < \gamma < 0$ give only more or less pronounced sharp peak at the critical point (the dependence is nonanalytical) of the isothermal susceptibility. In general, the $L \times 2$ RSRG transformations fail to reproduce the weak logarithmic singularities of the specific heat and isothermal susceptibility (at AF critical point). Of course, the above mentioned behavior is rather specific one and it is a hard task for any method to obtain logarithmic singularity.

Using the RSRG method we explored the phase diagram of a square antiferromagnet in an external magnetic field and the corresponding phase diagram of a lattice gas on a square lattice with repulsive nearest neighbor interactions. The critical temperature, the critical magnetic field and the critical surface coverage at $T = 0$ coincide rather well with the known values for these parameters. We calculated adsorption isotherms for different temperatures, the coverage dependences of the pair correlation function for nearest neighboring adparticles, the isothermal susceptibility and the chemical diffusion coefficient for different temperatures with and without considering interactions in the activated state of a nearest neighbor jump. These quantities have been compared to corresponding Monte Carlo data. The agreement between these results obtained by quite different methods is surprisingly good. Therefore, we can conclude that the RSRG method appears to be a rather reliable method which can be used to characterize the thermodynamic and kinetic properties of interacting adsorbates systems.

This work has been supported by the Heisenberg program of the Deutsche Forschungsgemeinschaft, by the International Association for the promotion of cooperation with scientists from the New Independent States of the former Soviet Union INTAS-96-0533, by the Fonds der chemischen Industrie (FCI), by CONICET (Argentina), Fundación Antorchas (Argentina) and by the National Agency for Promotion of Science and Technology (APCyT, Argentina), Proy. PICT98 No. C-03-03232.

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