Application of the Monte Carlo coherent-anomaly method to two-dimensional lattice-gas systems with further-neighbor interactions

A. Patrykiejew*
Institut für Physik, Johannes Gutenberg Universität, 6500 Mainz, Germany

P. Borowski
Department of Chemical Physics, Faculty of Chemistry, Maria Curie-Skłodowska University, 20031 Lublin, Poland
(Received 19 June 1989; revised manuscript received 26 January 1990)

A Monte Carlo version of the coherent-anomaly method has been used to determine critical properties of a two-dimensional Ising ferromagnet with nearest- and next-nearest-neighbor interactions and of a series of two-dimensional lattice-gas systems of particles interacting via 6-12 Lennard-Jones potential. It has demonstrated that the method leads to quite accurate determination of critical temperature but is less successful when used to determine the values of critical exponents γ and ν.

I. INTRODUCTION

Recently, Suzuki and his co-workers[1-8] proposed a new theoretical approach for determining critical properties of lattice systems, the so-called coherent-anomaly method (CAM). This approach unifies the mean-field theory with the Fisher scaling concept.[9] The strategy used by Suzuki and his co-workers is opposite to that utilized in the renormalization-group (RG) method.[10,11] In the RG method one eliminates the short-range fluctuations and obtains the renormalized long-range fluctuation effects recursively, using various approximate schemes.[11,12-14] On the other hand, CAM takes into account the long-range effects first; it introduces a self-consistent field to express the effects of long-range correlations, and then it treats the short-range fluctuations explicitly. CAM is done by constructing a series of clusters of increasing size and evaluating the cluster properties explicitly. Then, the "true" critical point for the infinite system is obtained by extrapolating the results to the cluster of infinite size. The hitherto-published results[1-8] demonstrated that CAM gives quite satisfactory results for both static and dynamic critical phenomena. Of course, as the cluster size increases the amount of numerical calculations involved also rapidly increases. Numerical difficulties have also limited applications of CAM to systems with the nearest-neighbor interactions only. A possible way around these computational difficulties has been proposed by Katori and Suzuki[3] in the form of a Monte Carlo version of CAM (MCCAM). These authors have successfully applied MCCAM to the three-dimensional Ising ferromagnet.

In this work we present the application of CAM to two-dimensional (2D) lattice systems involving further-neighbor interactions. In particular, we consider two series of lattice systems. The first series consists of an Ising ferromagnet with nearest- and next-nearest-neighbor interactions on a square lattice. Here we consider the effects on the critical properties of the model that result from the changes in the ratio of coupling constants for the nearest- and the next-nearest-neighbor interactions. A primary aim of this series of calculations was to determine the effects of the next-nearest-neighbor interactions on the convergence of MCCAM by comparison of the results with other estimations.[15-18]

The second series of systems considered in this work consists of 2D lattice-gas systems of Lennard-Jones particles located on a square lattice. By changing the relative size of adsorbed particles and the surface lattice we can study the effect of dimensional incompatibility on critical properties. From both experimental[19-23] and theoretical[23-27] studies of adsorption of gases on crystalline solids it is known that the critical temperature reaches a maximum for the dimensional incompatibility close to zero. Taking into account that theoretical calculations of these effects have been based on a rather simple mean-field model[23] the results obtained must be treated with reserve. Here, we present preliminary results obtained for model systems on a square lattice, but in the future we intend to consider systems resembling experimentally studied[19-29] monolayer films of argon, krypton, and methane on lamellar halides of the general formula MeX_2.

The paper is organized as follows. In the next section we define the lattice-gas model considered here and introduce basic notation. Then, Sec. III presents basic ideas of CAM and MCCAM. In Sec. IV we describe briefly the simulation method. Finally, in Sec. V we present the results and final conclusions.

II. THE LATTICE-GAS MODELS

In this work we consider a two-dimensional lattice gas on a square lattice, described by the Hamiltonian

$$\mathcal{H}-\mu N=\sum_{\langle i,j\rangle}\phi_{ij}n_i n_j-\mu\sum_i n_i+\mathcal{H}^0\ , \tag{1}$$

where n_i is the occupation variable assigned to each site and $n_i=1$ (0) when the site i is filled (empty), ϕ_{ij} is the energy of interaction between the particles located on sites i

and j, μ is the chemical potential in the system of N particles, and $\mathcal{H}^0$ is a constant irrelevant to the problems considered here. Now, setting

$$n_i=(1-s_i)/2 \tag{2}$$

we can transform the Hamiltonian (1) into the Hamiltonian for the Ising model[28]

$$\mathcal{H}=-\sum_{\langle ij\rangle} J_{ij}s_is_j-H\sum_i s_i+\mathcal{H}^{0*}\ , \tag{3}$$

where

$$J_{ij}=-\phi_{ij}/4 \tag{4}$$

and

$$H=(\mu-\tfrac{1}{2}\sum_{j(\neq i)}\phi_{ij})/2\ . \tag{5}$$

We consider the following two choices of the parameters J_{ij}. The first set of systems is defined by assuming that the interaction range does not exceed the next-nearest-neighbor distance, i.e.,

$$J_{ij}=\begin{cases} J_{\mathrm{NN}}, & i \text{ and } j \text{ are the nearest neighbors} \\ J_{\mathrm{NNN}}, & i \text{ and } j \text{ are the next-nearest neighbors} \\ 0, & \text{otherwise} \end{cases} \tag{6}$$

and both J_{NN} and J_{NNN} are assumed to be positive (ferromagnetic regime).

The second choice of the parameters J_{ij} results from the assumption that the interaction between a pair of particles is modeled by the (6-12) Lennard-Jones potential, i.e.,

$$\phi_{ij}\equiv\phi(|\mathbf{r}_i-\mathbf{r}_j|)\equiv\phi(r_{ij})=4\epsilon[(\sigma/r_{ij})^{12}-(\sigma/r_{ij})^6]\ . \tag{7}$$

Now, setting the cutoff distance, $R_{\max}$, at $a\sqrt{5}$, where a is the surface-lattice constant, i.e., restricting the range of interactions to the fourth-nearest neighbors, we have

$$J_{ij}=\begin{cases} -\phi_{ij}/4, & \text{for } r_{ij}\le R_{\max} \\ 0, & \text{otherwise}\ . \end{cases} \tag{8}$$

In this work we confine the range of variation of σ by assuming that the nearest-neighbor interaction is nonrepulsive, i.e., we keep $\sigma\le a$.

III. THE COHERENT-ANOMALY METHOD

Inasmuch as detailed presentation of CAM was given in a series of papers by Suzuki and his co-workers,[1-4] we shall confine ourselves to the discussion of its main points. The basic idea of CAM is to consider a series of molecular clusters of increasing size (or a series of approximations), to evaluate the cluster properties exactly, assuming that the spins located at the cluster boundary are subject to the local self-consistent fields (mean fields) exerted by outer spins (not belonging to the considered cluster), and then to extrapolate the results to the infinite cluster. In this way one can extract information about

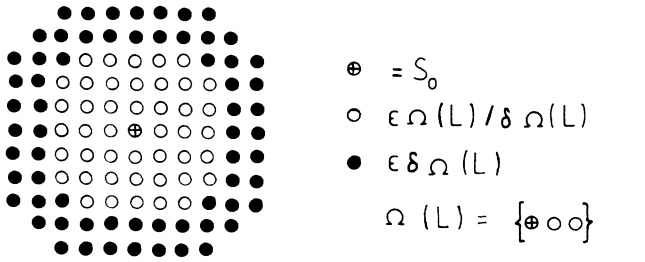

FIG. 1. An example of a cluster $\Omega(L)$ with the boundary region involving interactions up to the fourth-nearest neighbors.

the properties of macroscopic systems. The first step in CAM is to define the cluster. Let us consider the spin s_0 (or a particle located on a lattice site labeled by "0") and draw a circle of radius L with s_0 located in the center. All spins encompassed by this circle form a cluster $\Omega(L)$. Next, we define the boundary region of the cluster $\Omega(L)$, $\partial\Omega(L)$, by assigning any given spin to $\partial\Omega(L)$ if there is at least one spin outside the cluster $\Omega(L)$ interacting with this given spin. Of course, the size and width of the boundary region of the cluster depends on the assumed form of the Hamiltonian. Then, we split the Hamiltonian for the cluster (which includes the effects due to local self-consistent fields located outside of the cluster) as follows:

$$\mathcal{H}(L)=\mathcal{H}(\Omega(L))-H\sum_{i\in\Omega(L)}s_i-\sum_l J_l\sum_{k\in\partial\Omega(L)}s_kz_k^l\langle s\rangle\ , \tag{9}$$

where

$$\mathcal{H}(\Omega(L))=-\sum_l J_l\sum_{\langle ij\rangle_l\in\Omega(L)}s_is_j\ . \tag{10}$$

In the above, we have replaced J_{ij} by J_l, assuming that i and j are the lth nearest neighbors, whereas z_k^l is the number l-type bonds connecting the kth spin belonging to $\partial\Omega(L)$ with the outer spin [not belonging to $\Omega(L)$] (see Fig. 1).

It was demonstrated by Suzuki[2] that in order to determine the critical temperature for any cluster $\Omega(l)$ one must calculate the following "feedback" function (FBF):

TABLE I. Molecular clusters used in this work.

No.	L	N_L
1	1.50	9
2	2.50	21
3	3.90	45
4	4.90	69
5	5.60	97
6	6.90	145
7	7.99	193
8	8.99	249
9	10.99	373

$$\mathcal{F}(L,T)=\frac{J_{\mathrm{NN}}}{k_B T}\sum_{k\in\partial\Omega(L)} z_k^{\mathrm{NN}}\langle s_0 s_k\rangle_{T,\Omega(L)} , \tag{11}$$

where $\langle \ldots,\ldots\rangle_{T,\Omega(L)}$ denotes the average over the cluster, given by

$$\langle \mathrm{X}\rangle_{T,\Omega(L)} = \mathrm{Tr}\mathrm{X}\exp[-\beta\mathcal{H}(\Omega(L))]/\mathrm{Tr}\exp[-\beta\mathcal{H}(\Omega(L))] , \tag{12}$$

where $\beta=1/k_B T$, Tr is the usual trace operator and, in the present case $\mathrm{X}\equiv s_0 s_k$. Equation (11) is valid only for systems with the first-nearest-neighbor interactions.

In the present case of a Hamiltonian involving interactions between further neighbors, the feedback function $\mathcal{F}(L,T)$ takes the following form:

$$\mathcal{F}(L,T)=\frac{1}{k_B T}\sum_{k\in\partial\Omega(L)} C_k\langle s_0 s_k\rangle_{T,\Omega(L)} , \tag{13}$$

where

$$C_k=\sum_l z_k^l J_l . \tag{14}$$

Determination of the cluster critical temperature, $T_c(L)$, is based on the following equality:

$$\mathcal{F}(L,T_c(L))=1.0 . \tag{15}$$

Another quantity that must be evaluated in order to obtain information concerning critical properties of macroscopic systems is the classical susceptibility (χ_0). Above the cluster critical temperature, $T_c(L)$, the following relation holds:

$$\chi_0\simeq\bar{\chi}(T_c(L))\frac{T_c(L)}{J_1(T-T_c(L))}, \quad (J_1=J_{\mathrm{NN}}) , \tag{16}$$

where

$$\bar{\chi}(T_c(L))=\left[\frac{J_1}{k_B T}\frac{\sum_{i\in\Omega(L)}\langle s_0 s_i\rangle_{T,\Omega(L)}}{1-\frac{1}{k_B}\sum_{k\in\partial\Omega(L)} C_k\frac{\partial}{\partial T}\langle s_0 s_k\rangle_{T,\Omega(L)}}\right]_{T=T_c(L)} . \tag{17}$$

It can be readily demonstrated that the temperature derivative of the two-spin correlation function in Eq. (17) is represented by the four-spin correlation function, and in the present case we have

$$\frac{1}{k_B}\frac{\partial}{\partial T}\langle s_0 s_k\rangle_{T,\Omega(L)}=\left[\frac{1}{kT_B}\right]^2\left[\langle s_0 s_k\rangle_{T,\Omega(L)}\sum_l J_l\Big\langle\sum_{\langle ij\rangle\in\Omega(L)} s_i s_j\Big\rangle-\sum_l J_l\langle s_0 s_k\sum_{\langle ij\rangle\in\Omega(l)} s_i s_j\rangle\right] . \tag{18}$$

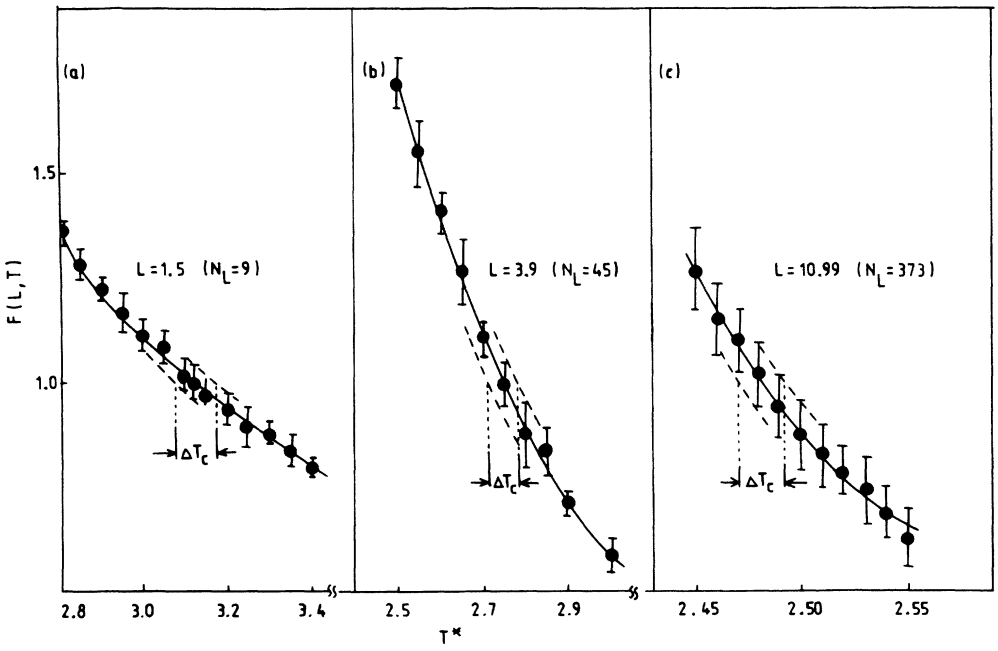

FIG. 2. Examples of temperature dependence of the function $\mathcal{F}(L,T)$ for a two-dimensional Ising ferromagnet with the first-nearest-neighbor interactions: (a) $L=1.5$ ($N_L=9$), (b) $L=3.9$ ($N_L=45$), and (c) $L=10.99$ ($N_L=373$).

TABLE II. Comparison of CAM and MCCAM results for a two-dimensional Ising ferromagnet.

Cluster No.	$T_c(L)$ Ref. 3	$T_c(L)$ This work	$\bar{\chi}(T_c(L))$ Ref. 3	$\bar{\chi}(T_c(L))$ This work
1	3.125 273	3.125 ∓ 0.030	0.403 176 1	0.402 ∓ 0.005
2	2.914 789	2.915 ∓ 0.027	0.479 064 2	0.481 ∓ 0.008
3	2.747 712	2.748 ∓ 0.018	0.584 701 3	0.587 ∓ 0.008
4	2.678 912	2.679 ∓ 0.014	0.644 048	0.644 ∓ 0.004
5	2.631 034	2.630 ∓ 0.010	0.696 316 8	0.709 ∓ 0.012
6	2.575 244	2.575 ∓ 0.010	0.778 271 8	0.782 ∓ 0.023
7		2.540 ∓ 0.008		0.845 ∓ 0.024
8		2.516 ∓ 0.006		0.902 ∓ 0.021
9		2.480 ∓ 0.006		0.962 ∓ 0.055

From CAM it follows that[1,2]

$$\lim_{L\to\infty} T_c(L)=T_c^* \ , \tag{19}$$

where T_c^* is the critical temperature of the macroscopic system, and the following scaling relations hold:

$$T_c(L)\simeq T_c^*+aL^{-1/\nu} \tag{20}$$

and

$$T_c(L)\simeq T_c^*+b\bar{\chi}(T_c(L))^{\gamma^{-1}} \ , \tag{21}$$

where ν and γ are the usual critical exponents associated with the correlation length and susceptibility critical behavior, respectively. We note, however, that L is not the best measure of the cluster size in the present case of pseudocircular clusters, since there always is a certain interval of L giving the same number of spins (or particles) in the cluster N_L. It is more accurate to replace the relation (20) by

$$T_c(L)\simeq T_c^*+a_1N_L^{-1/2\nu} \ , \tag{22}$$

where we have used the fact that

$$L\propto N_L^{1/2} \ . \tag{23}$$

The relations (21) and (22) can be used to extract the value of T_c^* as well as to estimate the values of the critical exponents γ and ν.

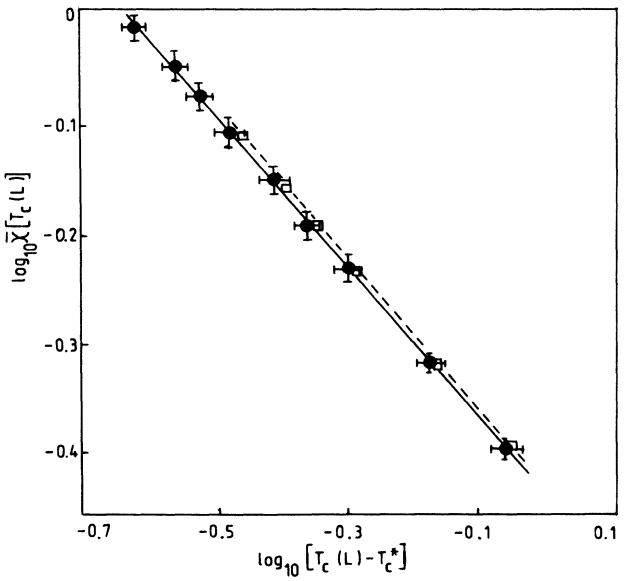

FIG. 3. Plots of $\log\bar{\chi}(T_c(L))$ vs $\log[T_c(L)-T_c^*]$ [Eq. (21)] for the two-dimensional Ising ferromagnet with the nearest-neighbor interactions obtained from CAM (Ref. 3) (open points) and MCCAM (solid points) calculations.

IV. MONTE CARLO PROCEDURES

In this work we have used a standard importance-sampling Monte Carlo method in grand ensemble.[29] First, the cluster of desired size was generated with the random starting configuration of its spins. Then, the system was equilibrated using 3000–5000 Monte Carlo steps per spin (MCS's). After equilibration, the next 10 000–15 000 MCS's were used to calculate averages. Only in a close vicinity of the cluster critical point [$\mathcal{T}(L,T)$ close to 1.0] longer runs were used with up to 40 000 MCS's. Each datum point was repeated five times using different starting configurations (achieved by changing the random-number-generator seed). Finally, mean values for each datum point were calculated. In this work we have used a series of nine clusters of size and number of spins given in Table I.

TABLE III. The critical parameters for the 2D Ising model.

	Exact value Ref. 31	CAM Ref. 3	MCCAM This work
T_c^*	2.269. . .	2.23 ∓ 0.038	2.245 ∓ 0.036
γ	1.75	1.785 ∓ 0.116	1.683 ∓ 0.083
ν	1.0		1.394 ∓ 0.117

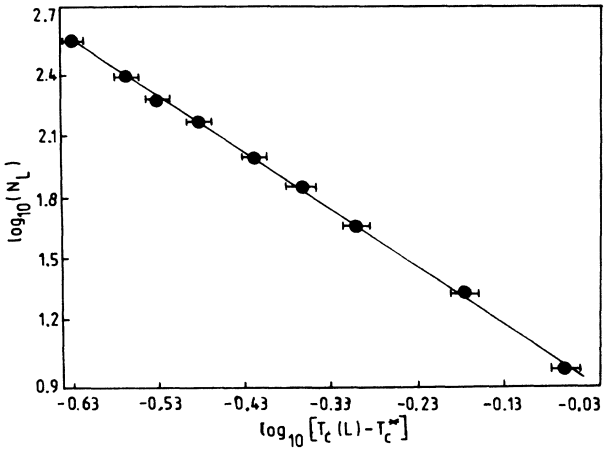

FIG. 4. The plot of $\log N_L$ vs $\log[T_c(L)-T_c^*]$ (Eq. 22) for the two-dimensional Ising ferromagnet with the nearest-neighbor interactions obtained from MCCAM calculations.

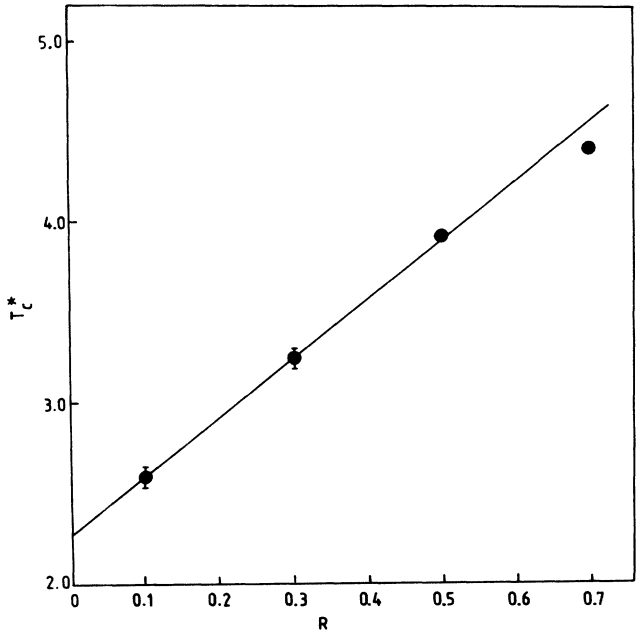

FIG. 5. The critical temperature for the two-dimensional Ising ferromagnet with the nearest- and next-nearest-neighbor interactions as a function of $R=J_{NNN}/J_{NN}$ calculated from Eq. (24) (solid line) and obtained from MCCAM calculations (points).

V. RESULTS AND DISCUSSION

The first series of calculations have been performed for a simple 2D Ising model with the nearest-neighbor interactions only. The exact values of the critical temperature and the critical exponents for this model are well known,[30,31] and hence this model can be conveniently used as a check for the method used here. In Fig. 2 we present examples of the temperature behavior of FBF for different cluster sizes. It is seen that as the cluster size increases the slope of the FBF in the vicinity of the cluster critical point increases also, so that $T_c(L)$ can be determined with high accuracy. In Table II we summarize the values of $T_c(L)$ and $\bar{\chi}(T_c(L))$ obtained by us and by Katori and Suzuki[3] with the help of analytic numerical CAM. It should be noted that for all clusters the values of $T_c(L)$ and $\bar{\chi}(T_c(L))$ obtained from CAM and MCCAM are practically the same.

The use of the scaling relation (21) to our results leads to quite an accurate value of the critical temperature but the critical exponent γ is a little lower than the exact value (1.75) (see Fig. 3 and Table III). On the other hand, the use of the scaling relation (22) with $T_c^*=2.245$ (see Fig. 4) leads to the value of the critical exponent ν considerably higher than the exact value (compare Table III). Next, in Table IV we present the results obtained for the model with nonzero second-nearest-neighbor interactions. From earlier theoretical studies[15–18] it is known that the critical temperature for this model exhibits the following dependence on $R=J_{NNN}/J_{NN}$:

$$T_c(R)=T_c(0)(1+\sqrt{2}R)\ , \tag{24}$$

whereas the critical exponent should remain the same as for a simple Ising model with the first-nearest-neighbor interactions.[32] In Fig. 5 we show a comparison of critical temperatures obtained for different values of R with the values predicted by the above relationship (24). It is seen that MCCAM leads to quite satisfactory results. The critical exponent γ obtained with help of the scaling relation (21) shows rather systematic deviations towards a lower-than-expected value of 1.75. Also, the values of ν derived from our results and the scaling relation (22) show a systematic shift towards higher values than the exact value $\nu=1.0$. The preceding results demonstrate that addition of the second-nearest-neighbor interactions does not affect the convergence of the method and gives results consistent with results obtained for simple model

TABLE IV. Critical parameters for 2D Ising ferromagnet with the second-nearest-neighbor interactions.

$J_{NNN}J_{NN}$	0.1	0.3	0.5	0.7
T_c	2.586∓0.022	3.235∓0.018	3.915∓0.016	4.400∓0.023
γ	1.641∓0.025	1.601∓0.031	1.535∓0.022	1.649∓0.018
ν	1.326∓0.053	1.278∓0.069	1.093∓0.062	1.357∓0.085

TABLE V. Critical parameters for 2D lattice-gas systems of Lennard-Jones particles of different relative size (σ/a).

σ/a	T_c^* ($=k_B T_c/\epsilon$)	γ	ν
0.800	0.580 ∓ 0.011	1.623 ∓ 0.090	1.224 ∓ 0.113
0.825	0.650 ∓ 0.015	1.771 ∓ 0.060	1.308 ∓ 0.125
0.850	0.735 ∓ 0.018	1.601 ∓ 0.160	1.182 ∓ 0.173
0.875	0.795 ∓ 0.019	1.611 ∓ 0.110	1.212 ∓ 0.152
0.900	0.820 ∓ 0.010	1.697 ∓ 0.120	1.197 ∓ 0.210
0.925	0.815 ∓ 0.006	1.747 ∓ 0.101	1.304 ∓ 0.167
0.950	0.780 ∓ 0.016	1.761 ∓ 0.085	1.115 ∓ 0.125
0.975	0.655 ∓ 0.014	1.601 ∓ 0.210	1.010 ∓ 0.102
1.000	0.390 ∓ 0.013	1.590 ∓ 0.225	1.323 ∓ 0.211

with nearest-neighbor interactions only.

Next, in Table V we present the results obtained for 2D lattice gas systems of Lennard-Jones particles with different relative size σ/a, ranging from 0.8 to 1.0. As expected, critical temperatures exhibit behavior typical to systems with different dimensional incompatibility,[23] here defined as

$$I=(\sigma\sqrt[6]{2}-a)/a \ . \tag{25}$$

As it is seen in Fig. 6, T_c^* reaches maximum for $I\simeq 0.03$. From experimental studies on adsorption of gases on crystalline surfaces it follows[20–22] that the critical temperature in monolayer films reaches its maximum value for $I\in(0.00,0.05)$. Thus, our results agree very well with this experimental finding. The observed changes of critical temperature with the dimensional incompatibility is, of course, caused by changes in the interaction energies between particle when σ changes, and the location of maximum for T_c corresponds to the value of σ at which the particles interact most strongly. In Fig. 7 we present the dependence between the system critical temperature and the parameter $J_{\rm sum}$ defined by

$$J_{\rm sum}=0.5\sum_l J_l z^l \ , \tag{26}$$

where z^l is the number of lth-nearest neighbors. We observe that only systems with $\sigma=0.800$ and 0.825, i.e., those with the most negative dimensional incompatibility, do not obey the expected linear behavior. The estimations of critical exponents γ and ν (compare Table V) were, in general, also not very successful. The exponent γ exhibits deviations towards mean-field value ($\gamma_{\rm MF}=1.0$), though is some cases we have obtained values quite close to the exact result. The exponent ν shows high positive deviations from the exact value $\nu=1.0$ (all LJ systems considered here belong to the same universality class as the Ising ferromagnetic model).

Concluding, we can say that the MCCAM does not seem to be as good as other methods used in studies of critical phenomena, e.g., the finite-size scaling of conventional Monte Carlo results, phenomenological scaling of transfer-matrix results or renormalization-group method. However, it requires considerably less computational time than, say, the conventional Monte Carlo method, as

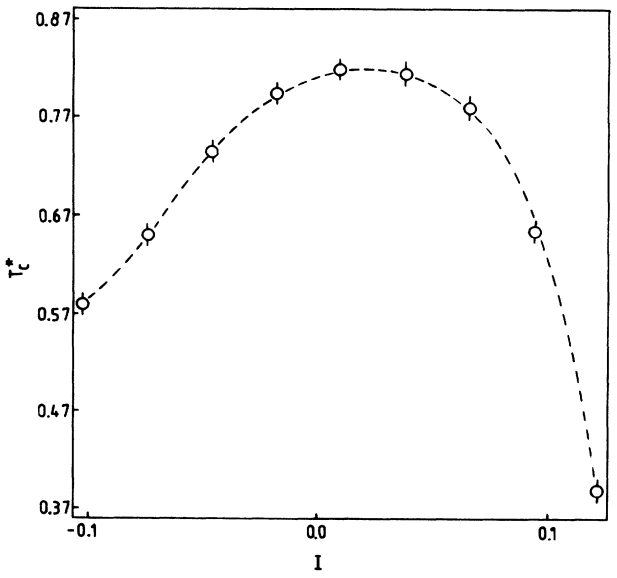

FIG. 6. The plot of critical temperatures of two-dimensional Lennard-Jones lattice-gas systems vs dimensional incompatibility I [Eq. (25)].

the cluster size increases then the effects of statistical fluctuations become more and more troublesome. In particular, in calculations of the susceptibility coefficients, $\bar{\chi}(T_c(L))$, the accuracy drops considerably as L increases. From our calculations it follows that for small clusters (with L up to 6.9) the error is of the order of 1% to 2%, whereas for large clusters (with L up to 10.99) this error can be as high as 10%.

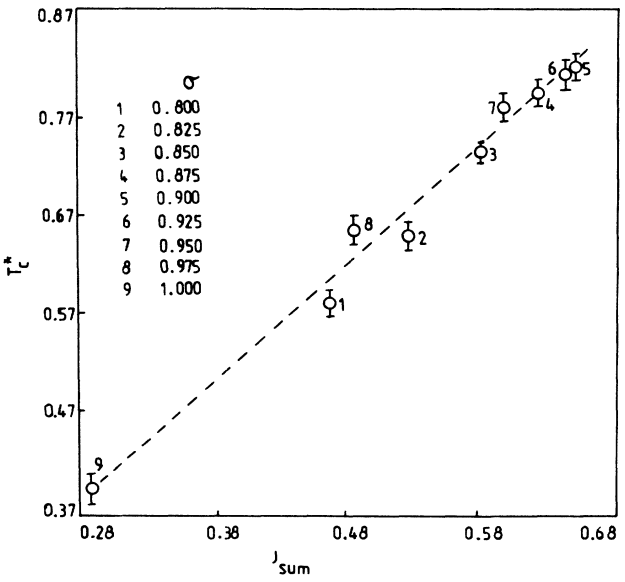

FIG. 7. Critical temperatures of two-dimensional Lennard-Jones lattice-gas systems as a function of the parameter $J_{\rm sum}$ [Eq. (26)].

ACKNOWLEDGMENTS

One of the authors (A.P.) wishes to express his thanks to Professor Kurt Binder (Institute of Physics, Johannes Gutenberg University, Mainz, Germany) for hospitality during his stay in Mainz and for very helpful and stimulating discussions. A.P. acknowledges financial support from the Alexander von Humboldt Foundation. This work was partially supported by the Central Program of Basic Research (CPBR), Poland, under Grant No. 01.08.

---

*Permanent address: Department of Chemical Physics, Faculty of Chemistry, Maria Curie-Skłodowska University, 20031 Lublin, Poland.

[1]M. Suzuki, J. Phys. Soc. Jpn. **55**, 4205 (1986).
[2]M. Suzuki, M. Katori, and X. Hu, J. Phys. Soc. Jpn. **56**, 3092 (1987).
[3]M. Katori and M. Suzuki, J. Phys. Soc. Jpn. **56**, 3113 (1987).
[4]X. Hu, M. Katori, and M. Suzuki, J. Phys. Soc. Jpn. **56**, 3865 (1987).
[5]X. Hu and M. Suzuki, J. Phys. Soc. Jpn. **57**, 791 (1988).
[6]M. Katori and M. Suzuki, J. Phys. Soc. Jpn. **57**, 807 (1988).
[7]M. Suzuki, Phys. Lett. A **127**, 410 (1988).
[8]M. Suzuki, Prog. Theor. Phys. Suppl. **87**, 1 (1986).
[9]M. E. Fisher, in *Critical Phenomena,* edited by M. S. Green (Academic, New York, 1971).
[10]K. G. Wilson, Phys. Rev. B **4**, 3174 (1971); **4**, 3184 (1971).
[11]S. K. Ma, *Modern Theory of Critical Phenomena* (Plenum, New York, 1975).
[12]L. P. Kadanoff, Ann. Phys. (N.Y.) **100**, 359 (1976).
[13]T. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1977).
[14]M. Schick, J. S. Walker, and M. Wortis, Phys. Rev. B **16**, 2205 (1977).
[15]N. W. Dalton and D. W. Wood, J. Math. Phys. **10**, 1271 (1969).
[16]D. P. Landau, J. Appl. Phys. **42**, 1284 (1971).
[17]G. Paul and E. Stanley, Phys. Rev. B **5**, 3715 (1972).
[18]S. Takase, J. Phys. Soc. Jpn. **36**, 636 (1974).
[19]Y. Larher, Ph.D. thesis, University of Paris, 1970.
[20]A. Enault and Y. Larher, Surf. Sci. **62**, 233 (1977).
[21]Y. Nardon and Y. Larher, Surf. Sci. **42**, 299 (1974).
[22]M. Matecki, A. Thomy, and X. Duval, Surf. Sci. **75**, 142 (1978).
[23]A. Patrykiejew and M. Jaroniec, Adv. Colloid Interface Sci. **20**, 273 (1984).
[24]A. Patrykiejew, Thin Solid Films **88**, 359 (1982).
[25]A. Patrykiejew, Thin Solid Films **105**, 259 (1983).
[26]D. K. Fairbent, W. F. Saam, and L. M. Sander, Phys. Rev. B **26**, 179 (1982).
[27]P. A. Monson, W. A. Steele, and D. Henderson, J. Chem. Phys. **74**, 6341 (1981).
[28]*Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer, Berlin, 1979).
[29]K. Binder, *Applications of the Monte Carlo Methods in Statistical Physics* (Springer, Berlin, 1984).
[30]L. Onsager, Phys. Rev. **65**, 117 (1944).
[31]H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Clarendon, Oxford, 1971).
[32]L. P. Kadanoff, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 5a.