Critical activity of the hard-sphere lattice gas on the body-centred cubic lattice

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Abstract
This is the first Monte Carlo study of the hard-sphere lattice gas with nearest-neighbour exclusion on the body-centred cubic lattice. We estimate the critical activity to be $0.7223 \pm 0.0003$. This result confirms that there is a re-entrant phase transition of an antiferromagnetic Ising model in an external field and a Blume-Emery-Griffiths model on the body-centred cubic lattice.
1 Introduction

For phase transitions and critical phenomena of a hard-sphere lattice gas [1, 2, 3] while many authors have investigated two-dimensional systems [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16], there are only a few studies in three dimensions [8, 17, 18]. One of the reasons is that series expansions or transfer matrix methods have been applied to the systems mainly. We have obtained the critical activity and the critical exponents of the hard-sphere lattice gas on the simple cubic lattice by using a Monte Carlo method and a finite-size scaling [17, 18]. In this paper we perform Monte Carlo simulations on the body-centred cubic lattice for the first time and estimate the critical activity.

Consider a hard-sphere lattice gas whose atoms occupy sites of a lattice and interact with infinite repulsion on a site and of nearest neighbour pairs. The grand partition function is

$$\Xi_V(z) = \sum_N z^N Z_V(N),$$

(1)

where $z$ is an activity and $Z_V(N)$ is the number of configurations in which there are $N$ atoms in the lattice of $V$ sites. At $z = +\infty$ a configuration of the ground state is that the atoms occupy all the sites of one sublattice and the other is vacant. There is no atom at $z = 0$. A continuous phase transition occurs at a critical activity.

The hard-sphere lattice gas relates to an antiferromagnetic Ising model in an external field [2, 9, 11]. The critical curve of the latter behaves as

$$H = H_c + a^* k_B T$$

near $T = 0$, where $T$ is the temperature; $H$ is the external field; $k_B$ is Boltzmann’s constant; $H_c$ is the critical field at $T = 0$. In the present paper we shall consider only the case $H_c > 0$. When $a^*$ is positive, a re-entrant phase transition occurs. The system is in the paramagnetic, the antiferromagnetic ordered, and the paramagnetic phase as $T$ is decreased when $H$ is fixed slightly above $H_c$. The slope, $a^*$, is given by the critical activity, $z_c$,

$$a^* = -\frac{1}{2} \ln z_c.$$ 

On the body-centred cubic lattice Gaunt [8] estimated $z_c$ to be 0.77(5) by using series expansions of the hard-sphere lattice gas and Landau [19] obtained $a^* = 0.160(16)$, i.e., $z_c = 0.726(23)$ from Monte Carlo simulations of
the antiferromagnetic Ising model. These results consist each other within errors. There is a re-entrant phase transition since $a^*$ is positive.

In the next section we define physical quantities measured. In section 3 we present Monte Carlo results. A summary is given in section 4.

2 Monte Carlo simulations

We use the Metropolis Monte Carlo technique [20, 21] to simulate the hard-sphere lattice gas (1) on the body-centred cubic lattice of $V$ sites, where $V = 2 \times L \times L \times L$ ($L = 2 \times n$, $n = 2, 3, \ldots, 12$), under fully periodic boundary conditions. A body-centred cubic lattice is made up two $L \times L \times L$ simple cubic lattices. According to Meirovitch [14], we adopt the grand canonical ensemble. The algorithm is described in the references [14, 17].

We start each simulation from a large activity and then gradually decrease an activity. The initial configurations have been obtained from preliminary simulations. The pseudorandom numbers are generated by the Tausworthe method [22, 23]. We measure physical quantities over $10^6$ Monte Carlo steps per site after discarding $5 \times 10^4$ Monte Carlo steps per site to attain equilibrium. We have checked that simulations from the ground state configuration and no atom one gave consistent results. Each run is divided into ten blocks. Let us the average of a physical quantity, $O$, in each block $\langle O \rangle_i$; $i = 1, 2, \ldots, 10$. The expectation value is

$$\langle O \rangle = \frac{1}{10} \sum_{i=1}^{10} \langle O \rangle_i.$$ 

The standard deviation is

$$\Delta\langle O \rangle = \left( \langle O^2 \rangle - \langle O \rangle^2 \right)^{1/2} / \sqrt{9}.$$ 

Let us define a density by

$$\rho = N/V$$

where $N$ is the number of the atoms in the lattice of $V$ sites and an order parameter by

$$R = 2 (N_A - N_B)/V$$
where \( N_A \) (\( N_B \)) is the number of the atoms in the A (B)-sublattice and \( N = N_A + N_B \). We measure the isothermal compressibility:

\[
\kappa = V \frac{\langle \rho^2 \rangle - \langle \rho \rangle^2}{\langle \rho \rangle},
\]

the staggered compressibility:

\[
\chi^\dagger = V \frac{\langle \langle \rho^2 \rangle - \langle |\rho| \rangle^2 \rangle}{4},
\]

and the fourth-order cumulant of \( R \):

\[
U = 1 - \frac{1}{3} \frac{\langle R^4 \rangle}{\langle R^2 \rangle^2}.
\]

### 3 Monte Carlo results

Figure 1 shows the activity dependence of the isothermal compressibility, \( \kappa_L(z) \), defined by (2) for various lattice sizes. The solid curves are obtained by the smoothing procedure of the B-spline. As \( L \) increases, the shape of the curve becomes sharper. There are shifts of the peak positions. In figure 2 we show the activity dependence of the staggered compressibility, \( \chi^\dagger_L(z) \), defined by (3) for various lattice sizes. It does not seem that the position of the peak shifts to contrast those of \( \kappa_L(z) \). We show the activity dependence of the fourth-order cumulant, \( U_L(z) \), of \( R \) defined by (4) for various lattice sizes in figure 3. There is an intersection between the curves with the size \( L \) and \( L + 2 \). The positions of these intersections are within a narrow region.

We define effective critical activities, \( z_{\kappa,max}^L \) and \( z_{\chi^\dagger,max}^L \), as the peak position of \( \kappa_L(z) \) and \( \chi^\dagger_L(z) \), respectively, and \( z_{U,\text{cross}}^L \) by

\[
U_L(z_{U,\text{cross}}^L) = U_{L+2}(z_{U,\text{cross}}^L).
\]

They will converge to the critical activity, \( z_c \), as \( L \to +\infty \). We plot them against \( 1/L \) in figure 4.

We decide to estimate \( z_c \) from \( z_{\chi^\dagger,max}^L \) by the following reasons. Although \( z_{\kappa,max}^L \) seems to behave systematically for \( L \geq 6 \), it is difficult to extrapolate \( z_c \) from it since we need a precise value of a critical exponent \( \nu \): \( z_{\kappa,max}^L - z_c \sim L^{-1/\nu} \). We do not know the value of this system. We cannot see systematic
behaviour in $z_{\chi^1}^\text{max}(L)$ and $z_{\text{cross}}^U(L)$ for $L \geq 8$. In the latter the value of $z_{\text{cross}}^U(20)$ is deviate from the others with $L \geq 12$. We can see from the definition (2) that it relates to the values of $z_{\text{cross}}^U(18)$ and $z_{\text{cross}}^U(22)$. Thus we do not adopt $z_{\text{cross}}^U(L)$ as an estimator of $z_c$ since we cannot ignore it simply. We get the result, $z_c = 0.7223(3)$, by the arithmetic mean from the data $z_{\chi^1}^\text{max}(L)$ with $L = 12, 14, \ldots, 24$. It consists with previous results, $z_c = 0.77(5)$ [8] and $z_c = 0.726(23)$ [11, 19], within errors. Our result is more precise than theirs.

4 Summary

We performed the Monte Carlo simulations of the hard-sphere lattice gas with nearest neighbour exclusion on the body-centred cubic lattice under fully periodic boundary conditions. We estimated the critical activity, $z_c$, to be $0.7223(3)$. It consists with $z_c = 0.77(5)$ by Gaunt [8].

As is described in section 1 the critical activity relates to the slope of the critical curve of the antiferromagnetic Ising model in the external field. Our result, $a^* = 0.1627(2)$, agrees with $a^* = 0.160(16)$ by Landau [19]. The system exhibits a re-entrant phase transition since $a^*$ is positive.

In closing this paper we want to mention that an antiferromagnetic Ising model in an external field is equivalent to a Blume-Emery-Griffiths model [26]. Kasono and Ono [27] confirms that there is a re-entrant phase transition of the latter on the body-centred cubic lattice. Our result supports theirs with high precision.

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Figure captions

Figure 1 Activity dependence of the isothermal compressibility, $\kappa$, defined by (2) of the hard-sphere lattice gas (1) on the body-centred cubic lattice of $V$ sites under fully periodic boundary conditions. $V = 2 \times L \times L \times L$; $L = 4$: ◊, 6: +, 8: □, 10: ×, 12: △, 14: *, 16: ○(small), 18: •(small), 20: ○(middle), 22: •(middle), 24: ○(large). The solid curves are obtained by the smoothing procedure of the fourth-order B-spline. The data with $L = 4, 6, \ldots, 14$ have been omitted to preserve the clarity of the figure.

Figure 2 Activity dependence of the staggered compressibility, $\chi^\dagger$, defined by (3). The meaning of the symbols and the curves is the same as in figure 1. The data with $L = 4, 6, \ldots, 20$ have been omitted to preserve the clarity of the figure.

Figure 3 Activity dependence of the fourth-order cumulant, $U$, defined by (4). The meaning of the symbols and the curves is the same as in figure 1. The data with $L = 4, 6, \ldots, 20$ have been omitted to preserve the clarity of the figure.

Figure 4 Size dependence of the effective critical activities, $z_{\kappa_{\text{max}}}(L)$: +, $z_{\chi^\dagger_{\text{max}}}(L)$: ○, and $z_{U_{\text{cross}}}(L)$: ×. Errors are less than the symbol size for $z_{\kappa_{\text{max}}}(L)$ and $z_{U_{\text{cross}}}(L)$. The horizontal line denotes $z = 0.7223$. 

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Figure 1

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Figure 2

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Figure 3

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Effective Critical Activity

Figure 4

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