A rejection-free Monte Carlo method for the hard-disk system

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We construct a rejection-free Monte Carlo method for the hard-disk system. Rejection-free Monte Carlo methods preserve the time-evolution behavior of the standard Monte Carlo method, and this relationship is confirmed for our method by observing nonequilibrium relaxation of a bond-orientational order parameter. The rejection-free method gives a greater computational efficiency than the standard method at high densities. The rejection-free method is implemented in a shrewd manner using optimization methods to calculate a rejection probability and to update the system. This method should allow an efficient study of the dynamics of two-dimensional solids at high density.

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I. INTRODUCTION

Monte Carlo (MC) methods have become more powerful tools with the development of faster and more accessible computers. Many different phenomena have been studied with MC methods [1, 2]. The melting behavior of the hard-disk system [3] is one of such subjects which has been studied with Monte Carlo methods [4, 5, 6, 7, 8, 9]. Consider the hard-disk system with \( N \) particles. The Monte Carlo method for the hard-disk system has the following steps. First, choose one particle randomly, i.e., choose it with a probability of \( 1/N \). Then choose a new position for the center of the chosen particle, the new position is chosen uniformly in the circle with radius \( \sigma_s \) centered on the original position of the particle. The trial move is accepted when the new position has no overlap with other particles, otherwise, the trial move is rejected.

The MC methods introduced above have been used to obtain the equilibrium state of the system. To study the equilibrium state of the system, the value of \( \sigma_s \), the trial step length, is often chosen in order that the rejection rate is near 50%. Recently, Watanabe et al. [10, 11] studied the hard-disk system by observing nonequilibrium behavior using a molecular dynamics (MD) method. In order to compare the results of MD and MC, we have to consider the dynamics of the MC method. The dynamics of the MC method for the hard-disk system can be understood as a Brownian motion, like pollen particles in a fluid. The value of \( \sigma_s \) corresponds to the amplitude of the external random force. Therefore, it determines a time scale of this system. If values of \( \sigma_s \) are not identical for all densities, we cannot compare the dynamics, like relaxation phenomena and fluctuations, between different densities. However, keeping \( \sigma_s \) fixed leads to high rejection rates in the Monte Carlo at high densities. A similar problem occurs for spin systems both at low temperatures and in a strong external field; a rejection rate becomes very high, so a huge number of trials is required to make a change. This problem can be avoided using a different technique called the rejection-free Monte Carlo (RFMC) method. The RFMC method was first constructed for discrete spin systems [12], for a review see [13]. Miyashita and Takano [14] applied the RFMC method to the kinetic Ising model in order to study dynamical critical behavior. Recently, Muñoz et al. [15] proposed a new RFMC algorithm which can treat models with continuous degrees of freedom. In this paper, we construct and utilize a RFMC algorithm for the hard-disk system based on the method of Ref. [15].

II. METHODOLOGY

A. A Rejection-free Monte Carlo method

\[
P(0|0) \equiv \lambda \\
P(1|0) \\
P(2|1) \\
P(N_s|0) \\
P(1|2) \\
P(0|0) \\
P(1|0) \\
P(2|1) \\
P(N_s|0)
\]

FIG. 1: A Markov chain of Monte Carlo steps.
A Monte Carlo method is an implementation of a Markov process on a computer, and hence is sometimes called a Markov Chain Monte Carlo. The Monte Carlo method calculates various physical quantities by updating states of a system using random variables. These updating processes can be illustrated by a Markov chain (see the schematic in Fig. 1). Let the current state be at $S_0$ and the states possible to move from $S_0$ are denoted by $S_i(i = 1, 2, \ldots, N_s)$. Define $E_i$ as the energy of the state $S_i$. The new state $S'_i(i = 0, 1, \ldots, N_s)$ will be chosen with probability $P(i|0)$. One way to ensure that the system will relax to the equilibrium state is to insist that the probability $P(i|0)$ satisfy the detailed balance condition.

One of the well-known ways to satisfy the detailed balance condition is to use a heat-bath transition probability. In the heat-bath method, the probability $P(i|0)$ is defined to be

$$P(i|0) = \frac{\exp(-\beta E_i)}{\sum_{k=0}^{N_s} \exp(-\beta E_k)}.$$  \hspace{1cm} (1)

When a system has a continuous degree of freedom, the summation of Eq. (1) becomes an integration which is generally difficult to calculate analytically.

Another popular way to satisfy the detailed balance condition is a Metropolis method. In this method, each step contains two parts; selecting a new state and accepting or rejecting the trial to move to the selected state. First, pick up a state $S_i$ from all possible states to move to with uniform probability $1/N_s$. The probability $P(i|0)$ to move from $S_0$ to $S_i$ is defined to be 1 when $\Delta E_i < 0$, otherwise it is $\exp(\beta\Delta E_i)$ with the energy difference $\Delta E_i \equiv E_i - E_0$. Therefore, the probability $P(i|0)$ in the Metropolis method is

$$P(i|0) = \begin{cases} 
1/N_s & \text{if } \Delta E_i \leq 0, \\
\exp(-\beta\Delta E_i)/N_s & \text{otherwise}. 
\end{cases} \hspace{1cm} (2)$$

When a trial is rejected, the configuration of the system is not updated. The probability $\lambda \equiv P(0|0)$ to stay in the current state after the trial is given by the expression

$$\lambda = 1 - \sum_{i \neq 0} P(i|0). \hspace{1cm} (3)$$

For some parameters, e.g. under a strong external field and at an extremely low temperature, the value of $\lambda$ can be very nearly 1. In such cases, most of computational time is spent on calculating trials which will be rejected. This rejection rate drastically decreases the efficiency of the computation.

In order to overcome this problem, a rejection-free Monte Carlo (RFMC) method is proposed. It is an example of an event driven algorithm [1, 2], and has also been called a waiting time method [13, 14]. Each steps of the RFMC method involves first computing the time to leave the current state (the waiting time $t_{\text{wait}}$), and then choosing a new state to move to with the appropriate probability. It does not contain the judgment to accept or reject a trial, and, therefore, it achieves rejectionless updates of the system in each algorithmic step. The waiting time $t_{\text{wait}}$ is calculated using a (pseudo) random variable. The probability $p(t)$ to keep staying at the current state for $t$ steps decays exponentially,

$$p(t) = \lambda^t = \exp(t \ln \lambda),$$  \hspace{1cm} (4)

with $\lambda$ defined in Eq. (4). Note that $\ln \lambda < 0$ since $0 < \lambda < 1$. Inversely, the time $t$ to stay in the current state is determined with a uniform random number $r$ on $(0, 1)$ to be

$$t_{\text{wait}} = \left\lfloor \frac{\ln r}{\ln \lambda} \right\rfloor + 1, \hspace{1cm} (5)$$

where $\lfloor x \rfloor$ denotes the integer part of $x$ and the rounding down is introduced to express the discrete time step in MC [13, 14].

After the time of the system is advanced by $t_{\text{wait}}$, a new state $S_i$ is chosen from the all states possible to move to except for the current state with the probability proportional to $P(i|0)$ [13, 14, 17]. Since all values of $P(i|0)$ are required to proceed one algorithm step in the RFMC, the computational cost of one step is higher than the normal MC. However, the waiting time $t_{\text{wait}}$, the time which can be advanced in one algorithmic step, becomes large at low temperatures, and consequently the efficiency of the RFMC can become better than that of standard MC.

### B. Application to hard-disk systems

Consider a hard disk system with $N$ particles with the radius $\sigma$. A standard MC method for the system involves choosing a particle, and trying to move the chosen particle within a circle with radius $\sigma_r$ centered on the original position of the chosen particle. To apply a RFMC method to the hard-disk system, define $\lambda_i$ as the probability that a trial to move particle $i$ is rejected (given that particle $i$ was chosen as the particle to attempt a move). Using the definition of $\lambda_i$, we can construct the algorithm of the RFMC method for the hard-disk system as follows:

1. Calculate the waiting time $t_{\text{wait}}$ using Eq. (5) with $\lambda = \frac{1}{N} \sum \lambda_i$.
2. Advance the time of the system by $t_{\text{wait}}$.
3. Choose a particle $i$ with the probability proportional to $1 - \lambda_i$, which is the probability that (given that particle $i$ was the particle chosen for an attempted move) the trial to move the particle $i$ would be accepted.
4. Choose the new position of the chosen particle $i$ uniformly from all the points to which the particle $i$ is allowed to move.
The steps described above are the same as the RFMC for continuous spin systems [13], but the algorithms to calculate $\lambda_i$ and to determine a new position of the chosen particle are unique to the hard-disk system. The probability $\lambda_i$ can be calculated to be,

$$\lambda_i = 1 - \frac{A_i}{\pi \sigma_s^2}, \quad (6)$$

with an area $A_i$ into which the particle $i$ is allow to move (see Fig. 2). Therefore, if we can calculate $A_i$ for all particles, then we can construct the RFMC algorithm for the hard-disk system.

FIG. 2: (Color online) A schematic drawing of the definition of $A_i$ (shaded). The solid circles are particles and the small dashed circle has a radius $\sigma_s$. The shaded area is the area which is a continuous set of the points that the center of the chosen particle can move to. The ratio of $A_i$ to the area of the trial circle $\pi \sigma_s^2$ gives the probability of accepting the move, $1 - \lambda_i$, given that the center particle has been chosen as the one to move.

C. Calculation of $A_i$

The area $A_i$ is the continuous set of positions in which the particle can be placed without any overlaps. Without neighboring particles, the shape of $A_i$ would be a filled circle with a radius $\sigma_s$. Let’s call it a trial circle. In the general case, the shape of $A_i$ is the remaining part of the trial circle after removing the overlap of ‘shadows’ of neighboring particles. The shape of the shadow is a circle with a radius $2\sigma$ which is concentric to a neighboring particle. Let’s call this a shadow circle. The area $A_i$, thus, consists of areas of arcs of a trial circle and that of shadow circles.

To compute the value of $A_i$, we develop a method we call the survival point method. See Fig. 3(a). The chosen particle is shown as a solid circle, the trial circle is shown as a concentric dashed circle, and the area $A_i$ is the shaded region. Each neighboring particle (filled circles) has a shadow circle which is concentric and has radius $2\sigma$. An enlargement of the area $A_i$ is shown in Fig. 2(b). It is seen that in this example this area has five vertices which are intersection points of shadow particles, we call them survived vertex points. In Fig. 2(c), these survived vertex points are shown as small filled circles. Straight lines connect the center of the chosen particle and the intersection points. In this case the area $A_i$ is divided into five figures.

Each divided figure is the remaining part of an isosceles triangle with the overlap of a shadow circle removed. It is easy to calculate this area. Thus, all we have to do is to find all survived vertex points which form the area $A_i$. First, make a list of all intersection points of shadow circles and the trial circle. Next, remove points which are included in other shadow circles from the list, since these points cannot be vertices forming the area $A_i$. After this removal process, we have the vertices which form the area $A_i$ (see Fig. 3(c)). The calculation process of a partial figure which forms $A_i$ is shown in Fig. 3(d). The vertices are denoted by $P_1$ and $P_2$, and the center of the shadow circle is denoted by $S$. The survived vertices $P_1$ and $P_2$ are on the shadow circle centered at $S$, so $SP_1 = SP_2 = 2\sigma$. The area of $OP_1SP_2$ can be calculated by summing the two triangles $OP_1P_2$ and $SP_1P_2$ with Heron’s formula. The area of the chord is $4\sigma^2 \theta$. Finally the portion of the area $OP_1P_2$ is calculated by subtracting the area of the chord $SP_1P_2$ from the area of the quadrilateral $OP_1SP_2$. The total area $A_i$ is the sum of one such calculation for each survived vertex.

D. Choosing a particle to move

After calculation of $t_{\text{wait}}$ and advancing the time of the system by it, we have to choose a particle $i$ to move with a probability proportional to $1 - \lambda_i$. With a direct implementation, i.e., with the integration scheme [13], the order of the computation is $O(N)$, which is very time consuming. Other approaches are proposed like a three level search for spin systems [19]. The three-level search improves the efficiency of the search by determining coordinates of a spin to update one by one. However, it is difficult to apply this method for particle systems, since neighbors of particles are not fixed. Here we use a complete binary tree search for the choosing part of the algorithm.

First, calculate the area $A_i$ for each of the particles. Since an acceptence probability $1 - \lambda_i$ is proportional to $A_i$ as shown in Eq. (6), the particle should be chosen with the probability proportional to $A_i$.

Next, construct a complete binary tree as follows,

1. Prepare a complete binary tree with enough height $h$, this height $h$ should satisfy $2h-2 < N \leq 2h-1$.

2. Label each node with $T^i_k$, which denotes the $n^{th}$ value at level $k$. The root node is labeled by $T^i_0$. 

has the sum of all $A_i$, that is,

$$T_k^h = \sum_i A_i. \quad (7)$$

Using this tree, we can choose a particle with the probability proportional to $A_i$ in the following way.

1. $k \leftarrow 1, i \leftarrow 1$.
2. Prepare a random number $r$ uniform on $(0, T_1^k)$.
3. $\begin{cases} i \leftarrow 2i-1 & \text{if } r < T_{2i-1}^k \\ i \leftarrow 2i & \text{otherwise} \end{cases}$
4. $k \leftarrow i - 1$.
5. if $k > 1$ then go to 2.

Consequently, choosing the bottom node requires $h - 1$ random numbers.

After the above processes, the final value of $i$ indicates the index of the particle to move. The order of this search algorithm is $O(\log N)$. When the position of particle $i$ is moved, the value of $A_i$ is also modified. We only have to update part of this tree for the chosen particle and its neighbors. The order of this update is also $O(\log N)$, which is much faster than $O(N)$ of the direct implementation. Details to implement the complete binary tree search method are described in the appendix.

A node labeled $T_{n}^{k+1}$ has branches leading to two nodes $T_{2n-1}^{k}$ and $T_{2n}^{k}$.

3. Associate every bottom node $T_1^j$ with the value of area $A_i$. If the number of bottom nodes $2^{h-1}$ is larger than $N$, the rest of the nodes are associated with zero, namely, $T_i^h = 0 \ (i > N)$.

4. Associate nodes at higher levels ($k > 1$) recursively with the sum of the values associated with its two children, namely, $T_{n}^{k+1} = T_{2n-1}^{k} + T_{2n}^{k}$.

A sample of a compete binary tree is shown in Fig. 4. Each node has the value $T_n^k$ and the value of each node at level $k+1$ is the sum of the values of its two children nodes at level $k$. The root node, which is $T_1^9$ in Fig. 4, has the sum of all $A_i$, that is,

$$T_k^h = \sum_i A_i. \quad (7)$$

Using this tree, we can choose a particle with the probability proportional to $A_i$ in the following way.

1. $k \leftarrow 1, i \leftarrow 1$.
2. Prepare a random number $r$ uniform on $(0, T_1^k)$.
3. $\begin{cases} i \leftarrow 2i-1 & \text{if } r < T_{2i-1}^k \\ i \leftarrow 2i & \text{otherwise} \end{cases}$
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have chosen to choose the new position using a Monte Carlo rejection method. Namely we generate a random position uniformly over some bounding area that includes all of the area $A_i$. [Such as the dashed circle of radius $\sigma$, in Fig. 3(a) or the rectangle in Fig. 3(c).] If this point is not in $A_i$ it is rejected and another uniformly distributed random point over the bounding area is generated. The first point not be rejected is the new position of the particle, since it is in the area $A_i$, and this point is used as the new center for the particle. This completes one algorithmic step of the RFMC method.

A value of area $A_i$ is very small compared to the trial circle at high density, and hence the Monte Carlo trial to find the new position of the particle to be moved became very inefficient. To improve this, it is effective to limit the trial area for the Monte Carlo by making the bounding area very close to the area $A_i$. We outline two different survived point methods, but have only implemented the first.

For the first method, the one actually implemented in this paper see Fig. 3(c). The solid rectangle is a bounding rectangle which includes the area $A_i$. It is easy to obtain the bounding rectangle with the survived vertex points. With the set of survived vertex points $\{(x_i, y_i)\}$, a diagonal line of the bounding rectangle is from $(\min\{x_i\}, \min\{y_i\})$ to $(\max\{x_i\}, \max\{y_i\})$. Then we can perform Monte Carlo trials for a new position within only this rectangle. The area of the rectangle is on the same order of $A_i$, so the probability of success to obtain the new position is drastically improved compared with the direct search over the trial circle.

An alternative method is first use a random number to decide which of the triangles formed with point O and two adjacent survived vertex points the survived point will fall into. This is done analytically since the area of each of these triangles with removed shadow circle chords have been already calculated. Then the shortest side formed with point O and the two survived vertex points (say $SP_2$ in Fig. 3(d)) is lengthened to be equal to the longest side ($SP_1$ in Fig. 3(d)). The random trial point is then generated within the section of the circle with a radius equal to the longest side ($SP_1$ in Fig. 3(d)). Then the point becomes the survived point used for the new location of point O if the trial point is within the shaded area. Otherwise, this procedure repeats in the same extended circular section until a survived point is found.

III. RESULTS

A. Calculation of $A_i$

In order to test our method to calculate $A_i$ described in Sec. II C, the values of $A_i$ were also evaluated by a Monte Carlo sampling ($A_{\text{MC}}$) with trial points uniformly drawn over the trial circle. The density of the system $\rho$ is defined to be $\rho = 4N\sigma^2/L^2$ with the number of particles $N$, the radius of the particles $\sigma$ and the linear system size $L$, respectively. Throughout this study, the number of particles $N$ is set to be 23288 and the periodic boundary condition is taken for both axes. The number of the generated configurations were 3000, and $10^6$ MC trial points are taken for each of the configurations to evaluate its area. The density of the system is fixed at $\rho = 0.9$. The result is shown in Fig. 3. The area $A_i$ is normalized by the area of the trial circles (see Fig. 3). An alternative method is first use a random number to decide which of the triangles formed with point O and two adjacent survived vertex points the survived point will fall into. This is done analytically since the area of each of these triangles with removed shadow circle chords have been already calculated. Then the shortest side formed with point O and the two survived vertex points (say $SP_2$ in Fig. 3(c)) is lengthened to be equal to the longest side ($SP_1$ in Fig. 3(c)). The random trial point is then generated within the section of the circle with a radius equal to the longest side ($SP_1$ in Fig. 3(c)). Then the point becomes the survived point used for the new location of point O if the trial point is within the shaded area. Otherwise, this procedure repeats in the same extended circular section until a survived point is found.

B. Time evolution

To compare the dynamics between the standard MC and the RFMC, we observed the time evolution of the six-fold bond-orientational order parameter $\phi_6$ [21]. The parameter $\phi_6$ is defined to be

$$\phi_6 = \langle \exp(i\theta) \rangle,$$  \hspace{1cm} (8)

with the bond angle $\theta$ which has a definition described in Fig. 3. The average is taken for all particle pairs of neighboring particles. The parameter $\phi_6$ becomes 1 when all particles are located on the points of a hexagonal grid, and it becomes 0 when the particle location is completely disordered. Therefore $\phi_6$ describes how close the system is to the perfect hexagonal packing. The neighbors in an off-lattice model are strictly defined with the Voronoi...
construction, which is a very time-consuming method. In this paper, two particles separated by a distance less than 2.6σ are defined as neighbors. We confirmed that the value of φ₀ is approximately the same value as the value obtained with the Voronoi construction. At the beginning of the simulation, the particles are set up in a perfect hexagonal order, namely, φ₀(𝑡 = 0, 𝜌) = 1. The order parameter φ₀ starts to relax to the value of the equilibrium state. With this nonequilibrium relaxation (NER) behavior of order parameters, critical points and critical exponents of various phase transitions can be determined accurately. This method is called a NER method. Watanabe et al. studied two-dimensional melting based on the NER method for the Kosterlitz-Thouless transition by observing the relaxation behavior of φ₀. Therefore, the following time evolutions of φ₀ contains information about the two-dimensional melting transition.

Time evolutions of φ₀ are shown in Fig. 7. Solid lines are results of the standard MC simulation and symbols (circles, triangles and squares) are the results of the RFMC. Fig. 7 shows that both behaviors are equivalent for the two methods. This is essentially a check of the program implementation, since the physical dynamic is the same for both the MC and the RFMC methods.

### C. Efficiency

The computational times required to achieve 1000 accepted MC steps are shown in Fig. 8(a). Configurations are started from the perfect hexagonal configuration and both measurements are started after 10⁷ MC steps. All simulations are performed on an Intel Xeon 2.4 GHz computer. While the computational time of the RFMC (open circles) is almost constant, a longer computational time is required for the standard Monte Carlo (solid circles) at higher density. It shows that the RFMC is more efficient at high densities, in spite of the additional bookkeeping involved in the RFMC method (so one algorithmic step takes much longer than one standard MC step).

The CPU-time ratio of the standard MC to the RFMC is shown in Fig. 8(b). The data are shown as a function of 1/ε, where ε = (ρ_{cp} − ρ)/ρ_{c}, the closest density is ρ_{cp} and the density of the system is ρ. The CPU-time ratio, which is the efficiency of the RFMC compared to that of the standard MC, diverges as ε⁻².

### IV. SUMMARY AND DISCUSSION

We constructed a rejection-free Monte Carlo algorithm for the hard-disk system. This method conserves the property of the dynamic behavior of the original Monte Carlo method. In other words, the time scales will not depend on the density, but are rather set by some Brownian-motion type of dynamic for all densities. An estimate of the time scales between the MC and physical time can thus be obtained by setting the mean-free path of an isolated particle to be proportional to the value σ_s. Note that strictly this is only true in the limit σ_s → 0, but it should be a reasonable approximation for a small finite σ_s.

We also find that for a fixed value of σ_s, the RFMC method is more efficient at high density. Therefore, the RFMC method should be useful for studies of two-dimensional solids or studies of high-density glass materials. It may also be possible to make the algorithm even more efficient by utilizing the ideas of absorbing Markov chains (for the MCAMC method for discrete state spaces see and references therein). Increased algorithmic efficiencies for the Monte Carlo dynamics of hard disks could be useful to further test physical phenomena using hard disk systems, such as for example the relationship between fluctuations and dissipation of work in a Joule experiment.
FIG. 8: (a) The required computational time to achieve 1000 acceptances of the Monte Carlo moves with the standard MC (open circles) and the RFMC (solid circles). (b) CPU-time ratio vs. $1/\varepsilon$ with $\varepsilon \equiv (\rho_{cp} - \rho)/\rho_{cp}$. Decimal logarithms are taken for both axes. The solid line is drawn for the visual reference ($C = 0.9 \times 10^{-3}$).

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Appendix

The complete binary tree search can be implemented with an one-dimensional array. To make it simple, let the number of particles $N$ be $2^h - 1$. The tree with height $h$ requires an array $a(i)$ with size $2N - 1$. First, associate each bottom node with a corresponding value as

$$a(N + i - 1) \leftarrow A_i \quad (i = 1, 2, \cdots, N), \quad (9)$$

which corresponds to $T^1_i \leftarrow A_i$. Next, associate parent nodes recursively as

$$i \leftarrow N$$

While $i \neq 0$

$$a(i) \leftarrow a(2i) + a(2i + 1)$$

$$i \leftarrow i - 1$$

next $i$

Using this array, we can pick up particle $i$ with the probability proportional to $A_i$ as,

$$i \leftarrow 1$$

While $i < N$

Prepare a uniform random number $r$ on $(0, a(i))$

$$\begin{cases} 
  i \leftarrow 2i & \text{if } r < a(2i) \\
  i \leftarrow 2i + 1 & \text{otherwise}
\end{cases}$$

next $i$

$$i \leftarrow i - N + 1.$$

After the above procedure, we obtain the index $i$ of the chosen particle. When the value of $A_i$ is changed, the tree should be updated. The update process is as follows,

$$a(N + i - 1) \leftarrow A_i$$

$$i \leftarrow \left\lfloor \frac{i + N}{2} \right\rfloor$$

While $i \neq 1$

$$a(i) \leftarrow a(2i) + a(2i + 1)$$

$$i \leftarrow \left\lfloor i/2 \right\rfloor$$

next $i$.

Note that, when the chosen particle is moved, the acceptance probabilities of the neighboring particles of the moved particle are also changed. Therefore, we have to perform the above process for all neighboring particles.
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