Monte Carlo simulations of a two-dimensional hard-disk boson system

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The ground-state properties of a two-dimensional hard-disk boson system at zero temperature were studied using a Monte Carlo method. The configurations were generated from trial Bijl-Jastrow-type wave functions for the fluid state and Nosanow-type wave functions for the solid state by the standard Metropolis random-walk algorithm. We found that the long-range-ordered crystal melts when the Lindemann ratio is greater than $\gamma_{\text{melting}}=0.279$. The corresponding fluid-solid phase-transition densities and pressure were determined to be $\rho_{\text{fluid}}=0.32\pm0.01$ and $\rho_{\text{solid}}=0.34\pm0.01$ and $P=7.3\pm0.3$ in reduced units. The physical picture emerging from the Monte Carlo results is discussed.

I. INTRODUCTION

This paper is concerned with the phase-transition properties of a hard-disk system at zero temperature. Besides the simplicity and relative transparency of the hard-disk system, which make it worthwhile in themselves to perform a detailed study, our interest in this subject was inspired by the recent experimental and theoretical progress in research on the magnetic flux lines in high-T_c superconductors.[1-3] Various regimes of the flux lines in high-T_c oxides and a two-dimensional interacting boson system were brought together by an elegant mapping relation through the isomorphism of the trajectories of vortices and boson world lines.[2] The partition function for classical flux lattice melting is approximately related to the S matrix in the study of quantum melting. The two-dimensional (2D) hard-disk boson system may also serve as a primary model to improve our knowledge on absorbed helium monolayers.[4-6] A better understanding on these typical two-dimensional (2D) boson systems will therefore provide some insight on many systems. Once this system is well understood, the remaining corrections, such as perturbation theory etc., to various systems can be introduced. It is the objective of the present paper to predict the transition densities between fluid and solid phases of the hard-disk boson system, and to illustrate some basic properties emerging from the simulations.

The most reliable and direct way to investigate a fluid-solid phase transition is to compute and compare the free energies for two phases. Once the free energies of the solid and fluid phases are determined, the fluid-solid equilibria are calculated by constructing common tangents in a Helmholtz free energy versus area diagram. Our procedure is based on an extension of the method used by Hansen, Levesque, and Schiff for a three-dimensional hard-sphere system[7] and therefore bears a lot of resemblance. In Sec. II we will model our system, introduce the variational wave functions, a Bijl-Jastrow-type wave function for the liquid phase a a Nosanow-type wave function for the crystalline phase, and briefly describe the procedure for evaluating the ground-state energy and pressure. The simulation results for the energy expectation values and pressures are also included in this section. We found that the system undergoes a first-order transition at densities $\rho_{\text{fluid}}=0.32\pm0.01(\sigma^{-2})$ and $\rho_{\text{solid}}=0.34\pm0.01(\sigma^{-2})$. We conclude with a discussion of our results in Sec. III. The reduced units have been used throughout this paper. That is, the unit of length is σ; the reduced densities is $\rho\sigma^2$, and energies are in units of $\hbar^2/2\mu\sigma^2$.

II. MONTE CARLO METHOD AND CALCULATION RESULTS

A collection of N hard-disk bosons of diameter σ and mass μ is described by the Hamiltonian

$$H=\sum_{i=1}^{N}-\nabla_i^2+\sum_{i<j}V(|\mathbf{r}_i-\mathbf{r}_j|)\ , \tag{1}$$

with

$$V(r)=\begin{cases}\infty & \text{if } r<1,\\ 0 & \text{otherwise.}\end{cases}$$

The Bijl-Jastrow wave functions that describe the ground state of the fluid phase were formulated in the same spirit of Hansen, Levesque, and Schiff:[7]

$$\Psi=\begin{cases}\displaystyle\prod_{i,j}\tanh\left[\frac{r_{ij}^m-1}{b^m}\right]=\prod_{i<j}f(r_{ij}) & \text{if } r>1\\ 0 & \text{otherwise,}\end{cases} \tag{2}$$

where m and b are two variational parameters and are determined by minimizing the total free energy for a given density.[7] This wave function gives the correct behavior when $r\le 1$ and $r\to\infty$, and is found to be quite good as a first approximation.[8] The long-range crystalline states were constructed by multiplying the Bijl-Jastrow wave function (2) by Gaussian factors $\prod_i\exp[-A(\mathbf{r}_i-\mathbf{R}_i)^2]$ centered at triangular lattice sites $\{\mathbf{R}_i\}$. This is the so-called Nosanow-type wave function. This function breaks the translational symmetry of the

trial wave function and localizes the particles on lattice sites, and hence describes a solid. The lack of symmetry with respect to particle interchange in this wave function should not be a major shortcoming since many simulations have indicated that several physical quantities, such as energy and pressure, etc., are not very sensitive to the symmetrization.[9,10]

The expectation values of the Hamiltonian for both liquid and solid state are obtained by virtue of the formula

$$E=\frac{\langle\Psi|H|\Psi\rangle}{N\langle\Psi|\Psi\rangle}=-\frac{\rho}{2}\int g(r)\nabla^2\ln f(r)d\mathbf{r}+3A\ , \quad (3)$$

where $g(r)$ is the pair distribution function.[11,12] Note that $A=0$ corresponds to a Bijl-Jastrow liquid state. This equation reduces our problem into the calculation of two-body correlation function $g(r)$. The relation between $g(r)$ and the variational wave function is

$$g(r)=\frac{N(N-1)\int\cdots\int|\Psi|^2dr_3dr_4\cdots dr_N}{\rho^2\int|\Psi|^2dr_1\cdots dr_N}\ . \quad (4)$$

For the crystalline state, the $g(r)$ used in (3) is an average over the orientation and different lattice sites. The formal analogy between this and a classical N-body system allows us to use a stochastic Monte Carlo method to attack this problem. In this approach, the sample configurations were generated from the trial wave functions by the Metropolis random-walk algorithm.[12,13]

All the computations reported here were on the ARDENT-Titan 3 minisupercomputer. We used a 90-particle system in a rectangular box of aspect ratio $5\sqrt{3}/9$, chosen to accommodate a perfect triangular lattice in high densities. We also did several runs on two larger systems, $N=224$ and 480, and we found that the size-dependent effect was negligible for the system. Starting from a random configuration for the liquid state and a triangular lattice for the crystalline state, we let the system approach equilibrium for the first 144 000 configurations and perform the averaging to obtain $g(r)$ over the next 144 000 configurations. The probability of accepting the trial configuration was adjusted to about 50% for every measurement.

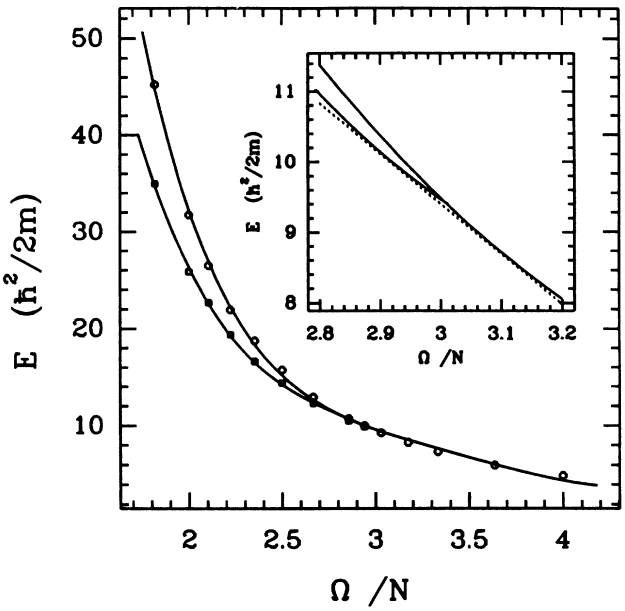

FIG. 1. Ground-state energy as a function of the area per particle. The circles and squares denote our measurements on the fluid and solid states respectively. The solid lines are fitted curves of the data to a polynomial. The inset represents the Maxwell double-tangent construction, which yields the phase transition densities $\rho_{\text{fluid}}=0.32\pm0.01$ and $\rho_{\text{solid}}=0.34\pm0.01$.

We show the measured curve of energy E versus area Ω in the region of phase transition in Fig. 1. The circles and squares denote our measurements on the fluid and solid phase, respectively. The solid lines are fitted curves of the data to a polynomial. In the inset of Fig. 1 we plotted the Maxwell double-tangent construction. The apparent discontinuity of curvature exhibited by the energy-versus-area plot suggest the existence of a domain of metastable state included between the two densities corresponding to the contact points of Maxwell double-

TABLE I. Variational results of the ground-state energy E and pressure P for both fluid and solid phases at different densities. The values of Lindemann's ratio γ for the solid phase, defined by rms deviation of a particle from its lattice site divided by the nearest-neighbor distance, is also tabulated.

	Fluid		Solid		
ρ	E	P	E	P	γ
0.200	3.14±0.03	1.5			
0.225	3.92±0.01	1.6			
0.250	4.90±0.04	2.5			
0.275	5.96±0.06	3.8			
0.300	7.33±0.05	5.3			
0.330	9.26±0.02	7.5			
0.340	10.00±0.03	8.6	9.88±0.08	7.3	0.279
0.350	10.71±0.06	9.4	10.51±0.02	8.0	0.266
0.375	12.93±0.06	13.6	12.28±0.02	10.6	0.253
0.400	15.73±0.09	18.1	14.38±0.07	14.1	0.238
0.425	18.76±0.16	22.3	16.61±0.10	18.3	0.222
0.450	21.94±0.14	28.1	21.39±0.04	22.8	0.213

tangent construction, a characteristic of a first-order phase transition. The double-tangent construction yields the transition densities $\rho_{\text{fluid}}=0.32\pm0.01$ and $\rho_{\text{solid}}=0.34\pm0.01$. The corresponding transition pressures were found to be $P=7.3\pm0.3$. The numerical results of the minimum energies and pressures are listed in Table I. In Table I we also listed the values of Lindemann's ratio γ for the crystalline state, i.e., rms deviation divided by the nearest-neighbor distance. It is seen that the solid melts when Lindemann's ratio γ is greater than 0.279, about 3 times larger than the value for a classical system, and is consistent with other quantum systems.[6,14] The pressures in the Table I were obtained by fitting the free energies to a polynomial of area Ω and then using the relation $P=-\partial E/\partial(\Omega/N)$. The overall error is estimated less than 8% on the pressure.

III. SUMMARY AND DISCUSSION

The fluid-solid phase transition of the system was marked by the fact that a long-range crystalline state, i.e., a Nosanow state with $A\neq0$, becomes energetically favorable at density $\rho=0.33$, and below the transition density it is the delocalized Bijl-Jastrow-type wave function (2), i.e., a Nosanow wave function with $A=0$, that optimizes energy. The pair correlation function $g(r)$, shown in Fig. 2, exhibits only a short-range order in the fluid just before freezing. The hard-disk boson system is is many ways similar to other quantum systems. No precursors of freezing, such as large fluctuations and surprisingly ordered liquid, etc., were observed before freezing. The crystallization of the system occurs at a much lower density in comparison with a classical hard-disk system; the classical hard-disk fluid is known to coexist with its crystal phase at a density $\rho=0.89$.[15] For a qualitative explanation of this fact, we refer readers to Ref. 7.

Dimensionality dependence of a quantum system is an important issue in simulation and experiment study. In the last two decades, extensive work has been done comparing two- and three-dimensional ^{4}He interacting via the Lennard-Jones potential.[16] It is instructive to compare our present results with those obtained for a 3D hard-sphere system. A 2D hard-disk fluid freezes at $\rho=0.32$, while the freezing density for a 3D hard-sphere system is only $\rho=0.23$.[17] The apparent difference between them disappears if we compare the mean particle separation at the freezing point. It is found that the mean particle separation $d_{2D}=2(1/\pi\rho)^{1/2}=2.00$, which is very close to the value for a 3D system, $d_{3D}=2(3/4\pi\rho)^{1/3}=2.02$. This is quite different from other quantum systems with a relatively "softer" interaction. For instance, Whitlock, Chester, and Kalos found that the particles are 22% farther apart in 2D helium than in 3D helium at the freezing point.[6] We speculate that for extremely hard core interactions, freezing occurs when mean particle separation is close to 2. In other words, a dimensional scaling of freezing exists for extremely hard core interactions. We attribute the apparent difference of the freezing densities between 2D hard-disk system and 3D hard-sphere system to this dimensional scaling. Whether this rough dimensional scaling can be extended to higher dimensions clearly deserves further investigation. We mention here that in analyzing the dimensional dependence of a system, the fact that a particle in a lower-dimensional system has fewer nearest neighbors might be important in some cases because the simplification of the configuration space would weaken the competitive ability of the interaction potential against the kinetic energy which tends to delocalize particles.

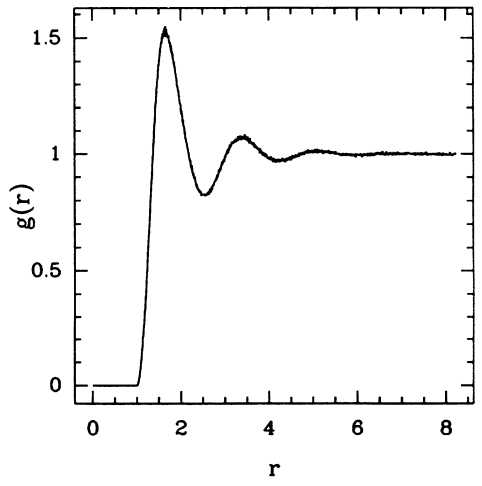

FIG. 2. Pair correlation function of the fluid state of the hard-disk boson system at the transition density $\rho=0.32$.

Properties of the 2D hard-disk boson system in the low-density limit have been investigated by Schick by summing ladder diagrams in the cluster development of the integral in power of the particle density.[4] The ground-state energy per particle was found to be $E=-4\pi\rho(\ln\rho)^{-1}[1+O(1/\ln\rho)]$. The method limits the validity of the results to very low densities and does not appear to be useful at the intermediate densities that are most interesting physically and where variational methods work. Nevertheless, for the sake of testing we did a few Monte Carlo runs at some fairly low densities to compare with Schick's formula. It turned out that they yielded close values.

The structure function $S(k)$, defined by

$$S(k)-1=\rho\int[g(r)-1]e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}$$
$$=2\pi\rho\int_0^\infty(g(r)-1)J_0(kr)r\,dr\ , \tag{5}$$

is an experimentally measureable function and can be easily obtained once $g(r)$ is known; here $J_0(x)$ is the zero-order cylindrical Bessel function. Conversely, one can obtain the pair correlation function from a known $S(k)$.[18] In Fig. 3 we plot the calculated structure factor of the system in the fluid state at the freezing density $\rho=0.32$. It would be most interesting to measure the structure factor in systems, such as absorbed helium monolayers etc., by using a neutron-scattering technique and make a comparison with the variational calculation. The dashed line in the small-k region in Fig. 3 is an artificial result according to Feynman's results $S(k)=\hbar k/2\mu s$,[19] where s is the velocity of sound. An in-

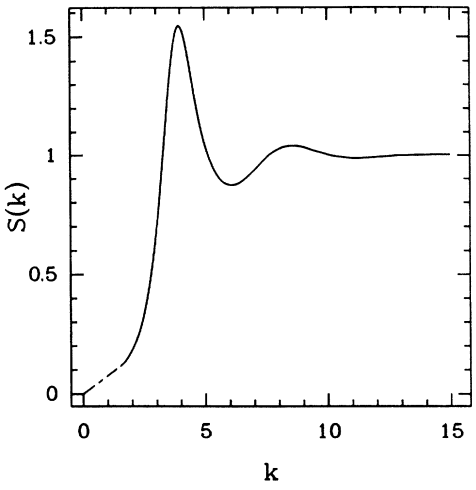

FIG. 3. Structure factor $S(k)$ of the fluid state of the hard-disk boson system at the transition density $\rho=0.32$.

corporation of the zero-point motion of long-wavelength long-range phonon modes is required to yield the linear behavior in the long-wavelength region in a variational calculation. The infinite-range correlation entails an inclusion of an additional product of pair function of infinite range in the wave function,[20] which would make the calculation much more involved.

The subject of a hexatic phase has long been an outstanding problem.[21] It is natural to ask whether there is a hexatic phase in a 2D quantum system. In fact, recent investigations on the flux lines in high-T_c superconductors has suggested the existence of a hexaticlike region followed by an entangled isotropic flux liquid region.[22] We have attempted to calculate the energy for the hexatic phase by using a variational function

$$\Psi=\prod_{i<j} f(r_{ij}) \prod_{i<j} \exp\left[\frac{a_3 \cos 6\theta_{ij}}{r_{ij}^{a_4}}\right], \tag{6}$$

where θ_{ij} is the angle between two particles i and j, a_3 and a_4 are two variational parameters in addition to the parameters in $f(r)$ given in Eq. (3). Unfortunately, we could not find any region where a hexatic phase is energetically favorable within our statistical errors. This, of course, does not rule out the possible existence of an intermediate hexatic phase. It is believed that the transition from a solid or a liquid phase to the hexatic phase is a second-order transition, i.e., the first-order fluid-solid transition being replaced by a succession of two "continuous" transitions. Therefore, in order to study the hexatic phase, one should seek other probes, such as derivatives of energy, other than energy itself. This work is still in progress.

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