Coexistence of Diagonal and Off-Diagonal Long-Range Order: A Monte Carlo Study

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The zero temperature properties of interacting two dimensional lattice bosons are investigated. We present Monte Carlo data for soft-core bosons that demonstrate the existence of a phase in which crystalline long-range order and off-diagonal long-range order (superfluidity) coexist. We comment on the difference between hard- and soft-core bosons and compare our data to mean-field results that predict a larger coexistence region. Furthermore, we determine the critical exponents for the various phase transitions.

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The possibility of a phase in dense Bose systems in which diagonal and off-diagonal long-range order (LRO) coexist has been the subject of discussion over the past 25 years [1,2]. Normally bosons at zero temperature are either superfluid (with off-diagonal LRO) or solid (with diagonal LRO). However, for a finite range of the interactions between the bosons a coexistence phase was predicted within a mean-field approximation [3–6]. This phase was interpreted in terms of Bose-Einstein condensation of vacancies in the solid, thereby forming a superfluid solid or supersolid. Experiments have been performed on ^{4}He, but no positive identification of this coexistence phase has yet been made. There are, however, strong hints towards such a phase [7]. On the theoretical side the discussion was restricted to the mean-field level. We are not aware of any more rigorous studies that identified a supersolid phase. In this Letter we report on Monte Carlo simulations of soft-core bosons on a square lattice in two dimensions that clearly demonstrate the existence of the supersolid phase beyond the mean-field approximation.

In general, lattice bosons are described by the Bose-Hubbard model [8]. In the limit where the average number of bosons per site is large, this model can be mapped exactly onto the quantum phase model which is in the same universality class. This model also describes Josephson junction arrays [9] in which the lattice sites are superconducting islands and the bosons are prefabricated Cooper pairs. The specific model we investigate is defined by the quantum phase Hamiltonian

$$H = \frac{1}{2}\sum_{ij} n_i U_{ij} n_j - \mu \sum_i n_i - t \sum_{\langle ij\rangle} \cos(\phi_i - \phi_j). \quad (1)$$

The number of excess bosons and the phase on site i are denoted by n_i and ϕ_i. Number and phase are conjugate variables that satisfy the commutation relation $[n_i, \phi_j] = i\delta_{ij}$. The hopping is written as a Josephson phase coupling, with matrix element t. The average density of bosons is controlled by the chemical potential μ. The interaction U_{ij} between bosons is chosen to be short range, i.e., on-site and nearest neighbor interactions, U_0 and U_1, only. A natural stability condition is that the number of nearest neighbors (four) times U_1 has to be smaller than U_0. The properties of the model (1) are periodic in $n_0 = \mu / \sum_i U_{ij}$ with period 1.

To gain understanding of the zero temperature properties of the model described by the Hamiltonian (1), we first discuss the mean-field phase diagram that is obtained following the method of Roddick and Stroud [6]. The phase diagram is shown in Figs. 1 (a) and 1(b) for U_1/U_0=0.125 and 0.2, respectively [10]. It is periodic in n_0 with period 1 and symmetric around $n_0 = \frac{1}{2}$. We discern four different phases: the superfluid phase (I), two incompressible Mott-insulating phases (II and III), and a compressible supersolid phase (IV). Phases I and IV have a nonzero superfluid stiffness ρ_0. Phases III and IV have nontrivial crystalline order ("checkerboard"; see the insets to Fig. 1) and therefore a nonzero (π,π) component of the static structure factor S_π. Thus, in the supersolid phase nontrivial diagonal LRO ($S_\pi \neq 0$) and off-diagonal LRO ($\rho_0 \neq 0$) coexist. In this phase the macroscopic wave function that ensures superfluidity is modulated on a short distance in order to reduce the interaction energy.

The phase diagram for hard-core bosons was investigated in Refs. [3–5]. In that limit a supersolid phase is possible only in the presence of *next* nearest neighbor interactions. The difference with soft-core bosons is the lack of multiple occupation. Indeed, the expectation value for two soft-core bosons to be at the same site is nonzero in phase IV in Fig. 1 [11]. We conclude that the possibility for bosons to hop over or past each other enhances the supersolid phase.

The points marked α, β, and γ in Fig. 1 have particle-hole symmetry. This means that the cost in interaction energy is the same for adding or removing a boson. Point α and the phase boundary between phases I and II were investigated in Refs. [8,12]. Point α and the line separating phases I and II have a different dynamical critical exponent z. This exponent determines the space-time asymmetry. The correlation length in the time direction diverges like $\xi_\tau \sim \xi^z$, if ξ is the correlation length in the space directions. Because of particle-hole symmetry the superconductor-insulator transition at point α has a dynamical critical exponent $z = 1$. The transition is in the

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3D XY universality class. For $n_0 \neq 0$ the transition has $z = 2$ and mean-field exponents apply. The same holds for point β and the line separating phases III and IV [12]. Motivated by these observations we also expect point γ to have $z = 1$, whereas for the transition at $n_0 \neq \frac{1}{2}$ from phase I to IV we expect $z = 2$. Below we show that this is consistent with our Monte Carlo data. The points marked δ in Fig. 1 have a first order transition, as the density jumps from 0 in phase II to $\frac{1}{2}$ in phase III.

Since fluctuations around the mean-field solution are likely to be important in two dimensions, one might wonder if the supersolid phase survives in an exact treatment. To investigate this question we performed Monte Carlo simulations of the model described by the Hamiltonian (1). We follow closely the method used by Sørensen *et al.* [13]. Thus, we map our two dimensional quantum model onto a three dimensional classical model of divergence-free current loops [we use the Villain form [14] for the cosine in Eq. (1); see Ref. [15] for a derivation]. The relevant quantity is then the partition function

$$Z = \sum_{\{J^\mu=0,\pm1,..\}} \exp\left\{-\sqrt{\frac{2}{K}}\left[\sum_{ij\tau}(J^\tau_{i,\tau}-n_0)\left(\delta_{ij}+\frac{U_1}{U_0}\delta_{\langle ij\rangle}\right)(J^\tau_{j,\tau}-n_0)+\sum_{i\tau,a=x,y}\left(J^a_{i,\tau}\right)^2\right]\right\}, \quad (2)$$

where the sum is over divergence-free discrete current configurations that satisfy $\nabla_\mu J^\mu = 0$ ($\mu = x, y, \tau$) and $\delta_{\langle ij\rangle}$ equals 1 for nearest neighbors and is 0 otherwise. The time components of the currents correspond directly to the particle numbers, $J^\tau_i = n_i$. The coupling constant $K = 8f\,t/U_0$, where the function f depends on the time-lattice spacing and the coupling. Here f is smaller than, but of the order of unity [11,14].

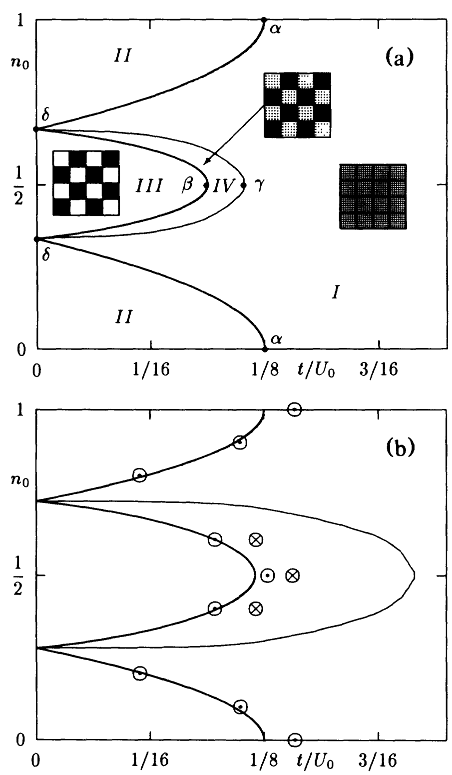

FIG. 1. Phase diagrams for soft-core bosons with on-site and nearest neighbor interaction. (a) U_1/U_0=0.125. (b) U_1/U_0=0.2. There are four different phases. I: superconductor; II: Mott insulating; III: Mott insulating with checkerboard charge order; and IV: supersolid. The points marked α, β, and γ have particle-hole symmetry. The points marked δ have a first order transition. The insets to (a) show the density distribution in the checkerboard, the supersolid, and the superfluid phases. In (b) the transition points from the Monte Carlo data are plotted as ⊙ and ⊗ for off-diagonal and diagonal LRO, respectively.

Using the standard Metropolis algorithm we generate configurations of currents in a system of size $L \times L \times L_\tau$ with periodic boundary conditions. We work in the grand-canonical ensemble at fixed n_0 in order to make contact to the phase diagrams in Fig. 1. As we are interested in a possible supersolid phase, the relevant quantities to measure are the superfluid stiffness for off-diagonal LRO and the structure factor for diagonal LRO.

In terms of the currents J^μ the superfluid stiffness (helicity modulus) is an average over loop configurations,

$$\rho_0 = \left\langle \frac{1}{L^2 L_\tau}\left|\sum_{i,\tau} J^x_{i,\tau}\right|^2\right\rangle. \quad (3)$$

The behavior near the transition satisfies the finite size scaling relation [16] $\rho_0 = L^{2-d-z}\tilde{\rho}(bL^{1/\nu}\delta, L_\tau/L^z)$ with $\tilde{\rho}$ a universal scaling function, b a nonuniversal scale factor, ν the coherence-length critical exponent, and $\delta = (K - K^*)/K^*$ the distance to the transition. At the critical point $K = K^*$, $\delta = 0$, and $L^z\rho_0$ is a function of L_τ/L^z only. Thus, plots of $L^z\rho_0$ vs K will intersect at the transition if L_τ/L^z is kept constant. Furthermore, the data for $L^z\rho_0$ plotted as a function of $L^{1/\nu}\delta$ for different system sizes should collapse onto one single curve. This allows the exponent ν to be determined. A similar scaling relation holds for the structure factor [17]

$$S_\pi = \left\langle \frac{1}{L^4 L_\tau}\sum_{ij,\tau}(-1)^{i+j} J^\tau_{i,\tau} J^\tau_{j,\tau}\right\rangle, \quad (4)$$

i.e., $S_\pi = L^{-2\beta/\nu}\tilde{S}(b'L^{1/\nu}\delta, L_\tau/L^z)$, with the order parameter exponent β. By a three parameter fit to the scaling relation for different system sizes the exponents ν and β as well as the critical coupling constant K^* are determined.

In the simulations we took U_1/U_0=0.2 in order to have a large coexistence phase. We performed simulations for

TABLE I. Critical couplings and exponents for the different transitions.

		The transition for				
		Off-diagonal LRO		Diagonal LRO		
n_0	z	K^*	ν	K^*	ν	β
0.5	1	0.775±0.005	0.65±0.08	0.837±0.005	0.55±0.05	0.21±0.04
0.4	2	0.645±0.008	0.44±0.08	0.749±0.006	0.5±0.1	0.25±0.10
0.2	2	0.446±0.005	0.5±0.1		For comparison:	
0.1	2	0.707±0.007	0.49±0.11	Mean-field:	1/2	1/2
0.0	1	0.843±0.005	0.61±0.08	3D XY:	2/3	1/3

constant n_0= 0.5, 0.4, 0.2, 0.1, and 0 and varied the coupling K. In the phase diagrams in Fig. 1 this corresponds to moving on horizontal lines through the phase transition(s). For n_0= 0.5 and 0 we simulated $L \times L \times L$ systems, where L= 6,8,10,12, as suggested by particle-hole symmetry and $z = 1$. Typically 100 000 sweeps through the lattice were needed for equilibration and the same amount for measurement. For n_0= 0.4, 0.2, and 0.1 we have $z = 2$. In order to keep the ratio L_τ/L^z constant, we simulated $L \times L \times L^2/4$ systems, where L= 6,8,10. For the largest system with L_τ= 25 we made up to 400 000 sweeps through the lattice for equilibration and the double for measurement. The results are summarized in Figs. 2–4 and Table I.

First we discuss our data for n_0=0.5. Figure 2 shows that there are two separate transitions for diagonal and off-diagonal LRO with a coexistence region in between where *both* the superfluid stiffness *and* the structure factor scale to a finite value in the thermodynamic limit. *This demonstrates the coexistence of diagonal LRO and off-diagonal LRO for soft-core bosons with nearest neighbor interaction in two dimensions.* In the neighborhood of the critical points the data fall onto a single curve when plotted as a function of $L^{1/\nu}\delta$ for a suitable choice of ν and β. An example is shown in Fig. 3. Table I shows that the exponent ν is different for the two transitions. For the transition related to superfluidity (point β in Fig. 1) we find a value for ν that is consistent with the 3D XY universality class. The universality class of the transition related to crystalline order (point γ) is not known.

Also at n_0=0.4 we find two separate transitions with different exponents that are the boundaries for the supersolid phase in between; see Table I and Fig. 4. The transition related to superfluidity (the line separating phases III and IV in Fig. 1) has ν ≈0.5 which is consistent with a mean-field transition in $d + z = 4$ effective dimensions. The transition related to crystalline order (between phases I and IV) has an order-parameter exponent β ≈0.25. This rules out a mean-field transition for diagonal LRO, although the transition is effectively four dimensional. In the neighborhood of this transition, fluctuations of the x, y components of the currents J induce long-range interactions for the τ components of the currents J [11]. It is likely that these long-range interactions are a relevant perturbation and suppress the exponent β.

Finally the data for n_0= 0.2, 0.1, and 0 are listed in Table I. Here there is only one phase transition, as the Mott-insulating lobes (phase II in Fig. 1) do not have any nontrivial crystalline order. Our data are consistent with a transition in the 3D XY universality class for n_0=0 and with a mean-field transition for n_0=0.1 and 0.2.

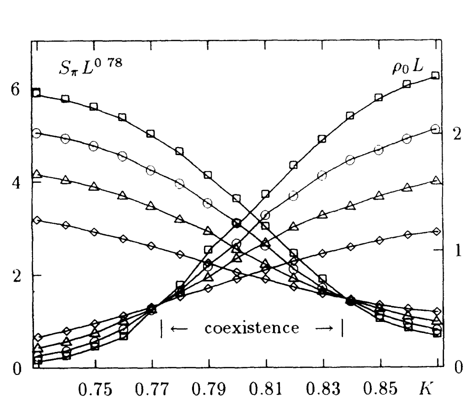

FIG. 2. Data for $L\rho_0$ and $L^{\frac{2\beta}{\nu}} S_\pi$ with $\frac{2\beta}{\nu}$=0.78 vs K at n_0=0.5. The curves cross at K^*=0.775 and 0.837, respectively. The region in between is the supersolid phase.

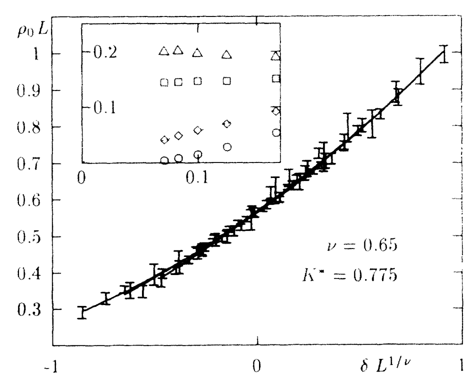

FIG. 3. Data for ρ_0 at n_0=0.5 in the neighborhood of the critical point at K^*=0.775. Plotted is $L\rho_0$ vs $\delta L^{1/\nu}$ with ν=0.65. Curves for different system sizes collapse onto a single curve. The drawn lines are a low order polynomial fit to the data. Inset: a plot of ρ_0 vs the inverse system size for K=0.86 (upper), 0.82, 0.775 (at the transition), and 0.74 (lower). The line is a guide to the eye.

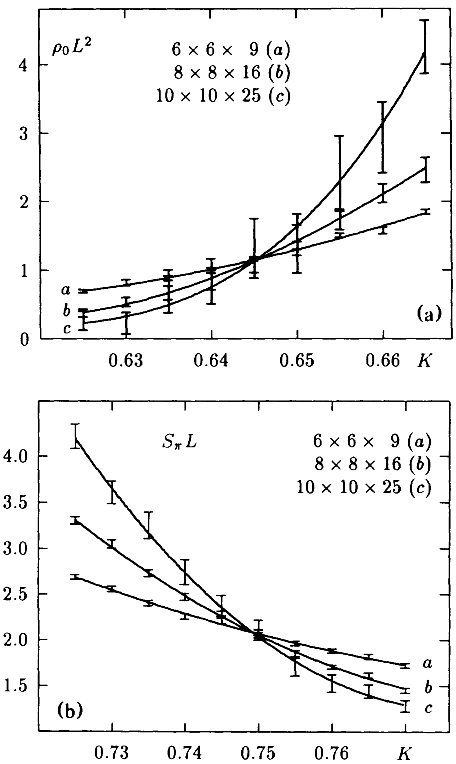

FIG. 4. Data for ρ_0 and S_π at n_0=0.4. The drawn lines are a low order polynomial fit to the data. (a) $L^2\rho_0$ vs K. The curves cross at K^*=0.645. (b) $L^{\frac{2\beta}{\nu}} S_\pi$ vs K with $\frac{2\beta}{\nu}$=1.0. The curves cross at K^*=0.749.

Using the explicit form of the function f that relates the coupling constants K and t/U_0, as given in Refs. [11,14], we compare in Fig. 1(b) the Monte Carlo data for the location of the phase transitions with the mean-field phase diagram. If the transition is mean field, the Monte Carlo data agree very well with the mean-field prediction. At the tips of the insulating lobes at n_0= 0 and 0.5, fluctuations reduce the superfluid phase as compared to the mean-field phase diagram. This makes the insulating lobes sharper, in accordance with the analysis of Ref. [18]. From Fig. 1(b) it is clear that mean-field theory overestimates severely the crystalline phase, and therefore the size of the supersolid phase.

In conclusion we have performed Monte Carlo simulations on soft-core lattice bosons in two dimensions that establish the existence of a supersolid phase in which diagonal and off-diagonal long-range order coexist. We estimated critical exponents as listed in Table I. The mean-field phase diagram of Ref. [6] is qualitatively confirmed. However, our simulations indicate that the supersolid phase is smaller than one would deduce from mean-field theory. We suggest that the coexistence phase may be observed in two dimensional systems such as Josephson junction arrays or thin ^{4}He films on suitable substrates. In these systems the possibility to vary the coupling constants as well as the chemical potential should make it possible to tune through the supersolid phase and see two sequential phase transitions.

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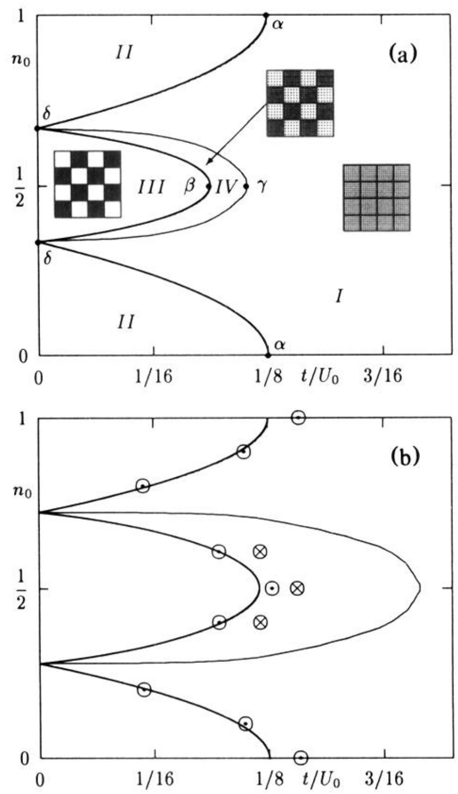

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