First Order Superconductor to Insulator Transition: Evidence for a Supersolid Phase

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The superconductor to insulator transition in the presence of long-range Coulomb interactions is studied using Monte Carlo techniques. At integer filling the transition is second order. At half filling we find evidence of a first order transition to a state with non-zero $S_{xx,x}$. No intervening supersolid phase is observed. Off half-filling two separate transitions are found. The transition from the superconducting to a supersolid phase is second order followed by another second order transition between the supersolid and an insulating phase.

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If a phase possesses both diagonal long range order (DLRO), associated with a structural ordering, as well as off diagonal long range order (ODLRO), indicating phase coherence, it is referred to as a supersolid. Initially Penrose and Onsager showed that such a phase cannot occur if each lattice site is always occupied. However, it was later realized that if the occupancy is not an integer, and if the wave-function is properly symmetrized, a supersolid phase can exist.\cite{1} Analogous phases in spin models were investigated and shown to be possible.\cite{2} Experimental evidence for a supersolid phase in solid \cite{3} and in recent experiments have been indications of novel behavior possibly related to a superhectic phase.\cite{4} Exploiting a duality argument\cite{5} the analogue of a supersolid phase of vortex lines in type-II superconductors has been proposed.\cite{6} Recent numerical studies have found evidence of supersolid phases in quantum lattice models\cite{7}. These studies indicate that interactions longer range than on-site are necessary to stabilize a supersolid phase. However, true long-range interactions were not considered, and the order of the transition was not investigated numerically.

In this communication we study the phase diagram of the 2D charged lattice Bose gas at several different filling factors. This model should be applicable to short coherence length superconductors where the individual Cooper pairs have formed prior to the superconducting transition.\cite{8} At integer fillings we find a second order transition with 3D XY-like exponents in agreement with predictions by Ma.\cite{9} At half-filling we find a single first order transition from the superconducting phase into an insulating phase with checkerboard charge ordering. No supersolid phase is found. Slightly below half-filling we find a second order transition from the superconducting phase into a supersolid phase with ODLRO and charge ordering followed by another second order transition into an insulating phase. A first order supersolid transition has recently been observed in a soft sphere model.\cite{10} A detailed account of our results will be published elsewhere.\cite{11}

Our starting point is the boson Hubbard model\cite{12,13,14}.

\begin{equation}
H = \frac{U}{2} \sum_r \hat{n}_r^2 - \sum_r (\mu - zt) \hat{n}_r - t \sum_{(r,r')} (\hat{\Phi}_r^\dagger \hat{\Phi}_{r'} + \hat{\Phi}_{r'}^\dagger \hat{\Phi}_r) + \frac{e^2}{2} \sum_{r,r'} \hat{n}_r G(r-r') \hat{n}_{r'}.
\end{equation}

Here $U$ is the on-site repulsion, $\mu$ is the chemical potential, $z$ the number of nearest neighbors, and $\hat{n}_r = \hat{\Phi}_r^\dagger \hat{\Phi}_r$ is the number operator on site $r$, with $\Phi_r^\dagger, \Phi_r$ boson creation and annihilation operators. The hopping strength is given by $t$ and $G$ is the $1/r$ Coulomb potential modified for the periodic lattice. We shall use either an Ewald or lattice Greens function for $G$ with $e^2 = 1/9$. This model can be mapped onto a link-current model\cite{15}.\cite{16} The integer-link variables are defined in terms of integer currents $J = (J^x, J^y, J^z)$ on the links of the $(2+1)$D lattice where $r = (x,y)$ and $\tau$ is the imaginary time which has been discretized. Note that $J^x$ is just the particle density. The integer-link variables $(J^x, J^y, J^z)$ take integer values from $-\infty$ to $\infty$, subject to the divergence-free constraint given by the continuity equation, $\nabla \cdot J = 0$. If we include long range Coulomb interactions we can write down a purely real action in this representation.\cite{17,18}

\begin{equation}
S = \frac{1}{K} \sum_{r,\tau} \left\{ \frac{1}{2} J^2(r, \tau) - \mu J^x(r, \tau) \right\} + \frac{e^2}{2K} \sum_{r,r',\tau} [J^x(r, \tau) - n_0] G(r-r') [J^x(r', \tau) - n_0].
\end{equation}

The calculation is performed in the canonical ensemble. Hence, the term involving $\mu$ is a constant and is only included for computational convenience. At integer filling in the absence of long-range interactions this model is in the same universality class as the 3D XY model and has an inverted XY transition.\cite{19,20,21}. Including long-range interactions previous studies have found that the transition can be either first or second order at integer filling.

Having arrived at an equivalent classical model we can employ standard Monte Carlo methods to study the insulating transition by letting $K$ take the place of a “temperature”. See Ref.\cite{12} for a detailed description. We
first locate the approximate position of the critical point, $K_c$, with low statistics calculations. Then the histogram Monte Carlo method is used to obtain high precision results for a range of $K$ close to $K_c$. For each system size $3 - 10 \times 10^4$ Monte Carlo sweeps (MCS) of the entire lattice are discarded for equilibration followed by $3 - 10 \times 10^4$ MCS for calculations with a measurement every 10 MCS. In order to calculate the error-bars we repeat the entire calculation 50 times for each lattice size. Two replicas with different random number sequences are run in parallel allowing overlaps between them to be calculated. Techniques used in the study of spin glasses then allow us to check that we are calculating equilibrium quantities. Thus we use in total $6 - 20 \times 10^6$ MCS to build the final distribution for use in the histograms.

In order to study the structural ordering we define the structure factor, $S_k$, as follows:

$$S_k = \frac{1}{L^d} \left< \left| \sum \sum e^{i k \cdot r} J(r, \tau) \right|^2 \right>.$$  (3)

Note that $S_k$ is positive definite. At half filling we expect the dominant ordering to be associated with the wave-vector $(\pi, \pi)$ corresponding to a checkerboard ordering with basis vectors $(a, a)$ and $(a, -a)$. The onset of the superconducting phase will be associated with a non-zero stiffness defined as

$$\rho = \frac{1}{L^d} \left< \left( \sum J(r, \tau) \right)^2 \right>.$$  (4)

Note that this stiffness corresponds to a non-zero Drude weight. Invoking finite-size scaling we arrive at the following finite-size scaling form for the stiffness

$$\rho = \frac{1}{L^{d+z-2}} L^{\nu} \left( \frac{\tau}{L^z} \right).$$  (5)

Here $z$ is the dynamical critical exponent defined through the relation $\xi_r \sim \xi^z$, and $\delta = K - K_c$ is the distance to the critical point, $K_c$. Assuming that the transition is second order, we see From Eq. (5) that if the aspect ratio, $c = L_\tau / L^z$, is kept constant $L^{d+z-2} \rho$ should be independent of $L$ at the critical point. In the presence of long-range Coulomb interactions Fisher et al. has argued that $z = 1$ and we shall in the following take that as our starting assumption.

**Integer filling.** For a filled lattice we do not expect any non-trivial charge ordering and there should only be a single transition between the superconductor and a Mott insulating phase, governed by a dynamical critical exponent $z = 1$. We therefore locate the critical point by calculating $L\rho$ using cubic samples. A well defined crossing is found at $K_c = 0.289(2)$. Using the finite size scaling form $L\rho = 0(\delta L^{1/\nu})$ a scaling plot of $L\rho$ can be used to determine $\nu$. We find $\nu \simeq 0.6$. We also calculate the correlation functions both in the time and space direction. This yields an independent calculation of the dynamical critical exponent, $z$, and the anomalous dimension $\eta$. By fitting the correlation functions at the critical point to power law forms we find $z = 1.0 \pm 0.1$, $\eta = -0.15 \pm 0.2$, in reasonable agreement with the prediction by Ma that the exponents should remain 3D-XY like due to the irrelevance of Coulomb interactions for this filling factor. However, critical amplitudes could possibly be affected by the Coulomb interactions and a priori we cannot expect to find the same value of the universal resistivity at the critical point as was found for the 3D-XY model. If we calculate the frequency dependent stiffness:

$$\rho(\omega_n) = \frac{1}{L^{d} \tau} \left< \left| \sum_{(r, \tau)} e^{i \omega_n \tau} J^2(r, \tau) \right|^2 \right>.$$  (6)

the conductivity can be calculated from the relation $\sigma(\omega_n) = 2\pi \rho(\omega_n) / \omega_n$. Here the quantum of conductance is $\sigma_Q \equiv (2e)^2 / h \equiv R_Q^{-1}$ and $\omega_n = 2m \pi / L\tau$ is the Matsubara frequency. With a $1/L$ finite size correction it is possible to collapse all the data for different lattice sizes onto a single curve at $K_c$ and we find $R_0 / R_Q = 1.5 \pm 0.4$.

**Half-integer filling.** We now turn to a discussion of the half filled case. In this case we presumably also have $z = 1$; however, none of the other exponents are known. In order to locate the structural transition associated with the assumed $(\pi, \pi)$ ordering we calculate a cumulant ratio of the structure factor $S_{\pi, \pi}$ defined as:

$$g(K) = (3 - S_{\pi, \pi}^2) / (S_{\pi, \pi}^2),$$

with this definition $g(K)$ should approach 1 in the ordered phase and 0 in the disordered phase. At the critical point $g(K)$ should be independent of $L$ and curves representing $g(K)$ for different lattice sizes should therefore intersect close to $K_c$ independent of the order of the transition. Our results are shown in Fig. 2 for the lattice sizes $L = 6, 8, 10, 12, 14$. The curves for different $L$ intersect at $K_c = 0.2559(4)$. However, above $K_c$ the curves for the larger $L$ develops a minimum and starts to increase. This behavior is usually associated with a first order phase transition. A plot of the probability distribution, $P(E)$ for the larger lattices shows a double peak structure close to $K_c = 0.2559(4)$. Following Lee and Kosterlitz we consider $A(E, L) \equiv -\ln P(E, L)$. Here $P(E, L)$ is calculated at $K_c(L)$, the coupling at which the probability distribution has two peaks of equal heights at $E = E_1, E_2$ surrounding a minimum at $E_m$. One can then define a bulk free-energy barrier between the ordered and disordered states as $\Delta F(L) = A(E_m, L) - A(E_1, L)$. In Fig. 2 we show results for $A(E)$ for $L = 8, 10, 12, 14.$ As a function of $L$, $\Delta F(L)$ increases monotonically. However, since $\Delta F(L)$ has not approached the asymptotic form $\Delta F(L) \sim L^{d+z-2}$ we expect that we in all cases have $L < \xi$, $S_{\pi, \pi}$ is significantly different in the two minima.

In Fig. 2 we show results for the cumulant ratio associated with the winding number and hence the onset of
superfluidity. This quantity as well as $L\rho$ shows that the superfluid order parameter disappears at the same $K_c$ where the first order structural transition takes place. We therefore conclude that the action Eq. (2) has a single first order phase transition at half-filling. We believe that this implies that the underlying quantum Hamiltonian therefore also has a first-order transition, although it is possible to argue that neglected irrelevant terms in Eq. (2) could cause the transition to be second order for the quantum problem. However, we have explicitly checked that the transition remains first order for both the Ewald and lattice Greens function form of the potential. The above scenario is in good agreement with recent work by Batrouni et al., and Scalettar et al.

Off half-filling. As the range of the interaction is increased a particulary rich phase diagram emerges for the boson Hubbard model. At half-filling the insulating phase at small $K$ corresponds to a checkerboard charge ordering with unit cell twice as large as the underlying lattice. Due to the limited lattice sizes that it is possible to study numerically, the most convenient filling factor away from half-filling is 7/16. At this filling factor we find, in the limit $K \to 0$, an insulating phase with charge ordering corresponding to vacancies in a $(0, 4a)$, $(4a, 2a)$, $(4a, -2a)$ triangular lattice superimposed on the half-filled $(\pi, \pi)$ ordering. Analogous orderings can be found at other filling factors. This charge ordering is commensurate with the lattice sizes $L = 8, 16$. Thus, at this filling factor we can use the $S_{\pi, \pi}$ structure factor to monitor any charge ordering even though the actual ground-state corresponds to ordering at more than one wave-vector. Scalettar et al. have shown that $z = 1$ at the superfluid-supersolid transition. Due to the long range interactions we expect $z = 1$ also at the supersolid-solid transition as opposed to the short-range case. In our simulations we therefore use $z = 1$ throughout. Our results are shown in Fig. 3. Two separate transitions are visible at $K_{c1} = 0.2125(15)$ and $K_{c2} = 0.2305(15)$ surrounding a supersolid phase. At the transition between the superconducting and supersolid phase we find $1/\nu \sim 1.8 \pm 0.3$. The transition between the supersolid and insulating phase is tentatively characterized by the exponent $1/\nu \sim 1.1 \pm 0.3$, but a detailed analysis is hindered by the fact that the $L = 12$ system is not commensurate with the assumed ground-state. We have also calculated the structure factors $S_{\pi, 0}$ and $S_{0, \pi}$ corresponding to collinear ordering. In none of the above cases have we observed charge ordering at these wave vectors.

In conclusion, we have found a first-order superconductor to insulator transition at half-filling. Off half filling we find evidence for a supersolid phase surrounded by two second order phase transitions.

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FIG. 1. The cumulant ratio of the structure factor, $S_{\pi,\pi}$, and winding number, $W$, as a function of $K$ at half-filling. The lines indicate results obtained using the histogram Monte Carlo method for different lattice sizes. The circles, squares and triangles denote separate calculations with lesser precision for lattices of size $L = 6, 8, 10$, respectively.

FIG. 2. $A(E) = -\ln P(E)$ as a function of $E/L^3$ for the lattice sizes $L = 8, 10, 12, 14$ at half-filling. $P(E)$ was calculated at $K_c(L) = 0.25345, 0.25465, 0.25504, 0.25548$, respectively. The relative height of the central peak increases with $L$.

FIG. 3. Results for a filling factor of 7/16. Shown are the the cumulant ratio for the structure factor, and $L\rho$ as a function of $K$. 