Quantum phase transitions from Solids to Supersolids in bi-partite lattices

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We studied some phases and phase transitions in an extended boson Hubbard model slightly away from half filling on bipartite lattices such as honeycomb and square lattice. We find that in the insulating side, different kinds of supersolids are generic stable states slightly away from half filling. We propose a new kind of supersolid: valence bond supersolid. We show that the quantum phase transitions from solids to supersolids driven by a chemical potential are in the same universality class as that from a Mott insulator to a superfluid, therefore have exact exponents $z = 2, \nu = 1/2, \eta = 0$ (with logarithmic corrections). Comparisons with previous quantum Monte-Carlo (QMC) simulations on some microscopic models on a square lattice are made. Implications on possible future QMC simulations are given.

1. Introduction: A supersolid is a state with both superfluid and solid order. Recently, by using the torsional oscillator measurement, a PSU’s group lead by Chan observed a marked $1 \sim 2\%$ Non-Classical Rotational Inertial (NCRI) even in bulk solid $^4$He at $\sim 0.2K$ [1]. The NCRI is a low temperature reduction in the rotational moment of inertia due to the superfluid component of the state [2]. If this experimental observation indicates the existence of $^4$He supersolid remains controversial [3, 4]. However, it was established by spin wave expansion [5] and quantum Monte-carlo (QMC) [3, 7, 8] simulations that a supersolid state could exist in an extended boson Hubbard model (EBHM) with suitable lattice structures, filling factors, interaction ranges and strengths. But so far, the universality classes of the quantum phase transitions from solids to supersolids have never been studied. This work, by using the dual vortex method developed in [13], we investigate some phases, especially supersolids and quantum phase transitions in an extended boson Hubbard model (EBHM) on bipartite lattices such as honeycomb and square lattice near half filling. Although the SS in lattice models is different from that in a continuous systems, the results achieved in this paper on lattice supersolids may still shed some lights on the possible microscopic mechanism and phenomenological Ginsburg-Landau theory of the possible $^4$He supersolids [1]. The EBHM in honeycomb and square lattices could be realized in ultracold atoms loaded on optical lattices. So the results achieved in this paper may have direct impacts on the atomic experiments.

The EBHM with various kinds of interactions, on all kinds of lattices and at different filling factors is described by the following Hamiltonian [10]:

$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + h.c.) - \mu \sum_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1)$$

$$+ V_1 \sum_{\langle ij \rangle} n_i n_j + V_2 \sum_{\langle\langle ik \rangle\rangle} n_i n_k + \cdots$$

(1)

where $n_i = b_i^\dagger b_i$ is the boson density, $t$ is the nearest neighbor hopping amplitude. $U, V_1, V_2$ are onsite, near-est neighbor (nn) and next nearest neighbor (nnn) interactions respectively, the $\cdots$ may include further neighbor interactions and possible ring-exchange interactions. A supersolid is defined as the simultaneous orderings of a microscopic approach such as Quantum Monte-Carlo (QMC) simulations on some microscopic models on a square lattice are made. Implications on possible future QMC simulations are given.

2. The dual vortex method. The dual approach is a MSG symmetry-based approach which can be used to classify some phases and phase transitions. But the question if a particular phase will appear or not as a ground state can not be addressed in this approach, because it depends on the specific values of all the possible parameters in the EBHM in Eqn.1. So a microscopic approach such as Quantum Monte-Carlo...
The effective action and order parameters in the dual vortex picture. The dual lattice of the honeycomb lattice is a triangular lattice. Two basis vectors of a primitive unit cell of the triangular lattice can be chosen as \( \vec{a}_1 = \hat{x}, \vec{a}_2 = -\frac{\sqrt{3}}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y}, \vec{a}_d = \vec{a}_1 + \vec{a}_2 \) as shown in Fig.1a. The reciprocal lattice of a triangular lattice is also a triangular lattice and spanned by two basis vectors \( \vec{k} = k_1 \vec{b}_1 + k_2 \vec{b}_2 \) with \( \vec{b}_1 = \hat{x} + \frac{\sqrt{3}}{2} \hat{y}, \vec{b}_2 = \frac{\sqrt{3}}{2} \hat{y} \) satisfying \( \vec{b}_1 \cdot \vec{a}_j = \delta_{ij} \). The point group of a triangular lattice is \( C_{6v} \sim D_6 \) which contains 12 elements. The two generators can be chosen as \( C_6 = R_{\pi/3}, I_1 \). The space group also includes the two translation operators along \( \vec{a}_1 \) and \( \vec{a}_2 \) directions \( T_1 \) and \( T_2 \). The 3 translation operators \( T_1, T_2, T_3 \), the rotation operator \( R_{\pi/3} \), the 2 reflection operators \( I_1, I_2, I_3 \), and the two rotation operators around the direct lattice points \( A \) and \( B \): \( R_{\pi/3} A \sim R_{\pi/3} B \) of the MSG are worked out in [13]. It can be shown that they all commute with \( \mathcal{H}_v \). However, they do not commute with each other, for example, \( T_1 T_2 = \omega T_3, T_3 T_1 = \omega^2 T_2 T_1 \), where \( \omega = e^{2\pi i/3} \).

In the following, we focus on \( q = 2 \) case [12] where there is only one dual vortex band \( E(\vec{k}) = -2t(t \cos k_1 \cos k_2 - \cos (k_1 + k_2)) \). Obviously, \( E(k_1, k_2) = E(-k_1, k_2) = E(k_2, k_1) \). There are two minima at \( \vec{k}_\pm = \pm (\pi/3, \pi/3) \). Let’s label the two eigenmodes at the two minima as \( \psi_{a/b} \).

The two fields transform under theMSG in the following way:

\[
\begin{align*}
\mathcal{L}_{\text{SF}} &= \sum_{\alpha=a/b} \left| (\partial_\mu - i A_\mu) \psi_\alpha \right|^2 + r |\psi_\alpha|^2 + \frac{1}{4e^2} (\epsilon_{\mu\nu\lambda} \partial_\mu A_\nu \partial_\nu A_\lambda - \gamma_0 (|\psi_a|^2 + |\psi_b|^2) - \gamma_1 (|\psi_a|^2 - |\psi_b|^2)^2 + \cdots
\end{align*}
\]

where \( A_\mu \) is a non-compact \( U(1) \) gauge field, \( r \) is a dimensionless constant depending on \( t, U, V_1, V_2 \cdots \) in Eqn[1]. Upto the quartic level, with correspondingly defined \( \psi_{a/b} \) in a square lattice, Eqn[2] is the same as that in the square lattice derived in [13].

Because the duality transformation is a non-local transformation, the relations between the phenomenological parameters in Eqn[2] and the microscopic parameters in Eqn[1] are highly non-local and not known. Fortunately, we are still able to classify some phases and phase transitions and make some very sharp predictions from Eqn[2] without knowing these relations. If \( r > 0 \), the system is in the superfluid state \( < \psi_1 >= 0 \) for every \( l = a/b \). If \( r < 0 \), the system is in the insulating state \( < \psi > \neq 0 \) for at least one \( l \).

In the insulating or supersolid states, there must exist some kinds of charge density wave (CDW) or valence bond solid (VBS) orders which may be stabilized by longer range interactions or possible ring exchange interactions in Eqn[1]. Up to an unknown prefactor \([15]\), we can identify the boson (or vacancy) densities on sites \( A \) and \( B \) and the boson kinetic energy on the link between \( A \) and \( B \) which are the order parameters for the CDW and VBS respectively as \( \rho_A = \psi_a^\dagger \psi_a, \rho_B = \psi_b^\dagger \psi_b \) and \( K_{AB} = e^{i \vec{Q} \cdot \vec{r}} \psi_a^\dagger \psi_b + e^{-i \vec{Q} \cdot \vec{r}} \psi_b^\dagger \psi_a \) where \( \vec{Q} = 2\pi/3(1,1) \) and \( \vec{x} \) stands for dual lattice points only. We assume \( r < 0 \) in Eqn[2] so the system is in the insulating state. In the following, we discuss the Ising limit first, then the easy-plane limit.

4. Phase diagram (a) Ising limit. If \( \gamma_1 > 0 \), the system is in the Ising limit, the mean field solution is \( \psi_a = 1, \rho_b = 0 \). The system is in the CDW order which could take checkboard \((\pi, \pi)\) order [16]. Eqn[2] is an expansion around the uniform saddle point \( < \nabla \times \vec{A} >= f = 1/2 \) which holds in the SF and the VBS (to be discussed in section 5 ). In the CDW state, a different saddle point where \( < \nabla \times \vec{A} >= -\alpha \) for sublattice \( A \) and \( < \nabla \times \vec{A} >= \alpha \) for sublattice \( B \) should be used. So the transition from the SF to the CDW is a strong first order transition. It can be shown [17] that there is only one vortex minimum \( \psi_b \) in such a staggered dual magnetic field with \( \alpha < 1/2 \), the effective action inside the CDW state is:

\[
\mathcal{L}_{\text{CDW}} = \left| (\partial_\mu - i A_\mu^0) \psi_b \right|^2 + r |\psi_b|^2 + u |\psi_u|^4 + \cdots + \frac{1}{4e^2} (\epsilon_{\mu\nu\lambda} \partial_\mu A_\nu^0 \partial_\nu A_\lambda - \gamma_0 (|\psi_u|^2 + |\psi_v|^2) - \gamma_1 (|\psi_u|^2 - |\psi_v|^2)^2 + \cdots
\]

where the vortices in the phase winding of \( \psi_b \) should be interpreted as the boson number [18]. The gauge field \( A^0 \) is always massive.

Eqn[4] has the structure identical to the conventional component Ginzburg-Landau model for a "superconductor" in a "magnetic" field. By a duality transformation back to the boson \( \Psi \) picture, it can be shown that the transition driven by \( \delta f \) is in the same universality class of Mott to superfluid transition which has the exact exponents \( z = 2, \nu = 1/2, \eta = 0 \) with logarithmic corrections first discussed in [10, 11]. This fact was used in [15] to show that for type II superconductors, the gauge field fluctuations will render the vortex fluid phase intruding at \( H_{c1} \) between the Messimer and the mixed phase Fig2a. For parameters appropriate to the cuprate superconductors, this intrusion occurs over too narrow an interval of \( H \) to be observed in experiments.

In the present boson problem with the nearest neighbor interaction \( V_1 > 0 \) in Eqn[1] which stabilizes the \((\pi, \pi)\) CDW state at \( f = 1/2 \), this corresponds to a CDW su-
persolid (CDW-SS) state intruding between the commensurate CDW (C-CDW) state at $f = 1/2$ and the incommensurate CDW (IC-CDW) state at $1/2 + \delta f$. The CDW-SS has the same lattice symmetry breaking as the C-CDW. (c) The Easy-Plane limit $\gamma_1 < 0$. There is a Valence Bond Supersolid (VB-SS) state intruding between the commensurate VB-SS state (C-VBS) state at $f = 1/2$ and the incommensurate VB-SS (IC-VBS) state at $1/2 + \delta f$. The VB-SS has the same lattice symmetry breaking as the C-VBS. The thin (thick) line is the 2nd (1st) order transition. The 1st order transition in the Ising (Easy-plane) limit is weakly (strongly) one.

< $\nabla \times \vec{A} > = f = 1/2$ holds in both the SF and the VBS, so the transition from the SF to the VBS is a weak first order transition. The system has a VBS order, the kinetic energy $K_{AB} = \cos(Q \cdot \vec{r} + \theta_\perp)$ where $\theta_\perp = \theta_a - \theta_b$. Upto higher order terms are needed to determine the relative phase. It was shown in [13] that there are only 3 sixth order invariants: $C_1 = |\psi_a|^6 + |\psi_b|^6, C_2 = (|\psi_a|^2 + |\psi_b|^2)|\psi_a|^2|\psi_b|^2, C_3 = (\psi_a^* \psi_b)^3 + (\psi_b^* \psi_a)^3 = \lambda \cos 3\theta_\perp$. Obviously, only the last term $C_3$ can fix the relative phase. It is easy to show that both signs of $\lambda$ are equivalent, in sharp contrast to the square lattice where the two signs of $C_{sq} = \lambda \cos 4\theta$ lead to either Columnar dimer or plaquette pattern. One VBS with $\lambda > 0, \theta_\perp = \pi$ was shown in Fig.1a. The other two VBS states can be obtained by $R^{\pm\pi/3}_{12}$. In contrast to the square lattice where $C_{sq}$ is irrelevant near the QCP, $C_3$ may be relevant, so the transition from the SF to the VBS in Fig.1b could be a 1st order transition. Slightly away from the half-filling, Eqn.2 becomes:

$$L_{VBS} = \frac{1}{2} (\partial_\mu \theta_a - A_\mu)^2 + \frac{1}{4e^2}(\epsilon_{\mu\nu\lambda}\partial_\mu A_\lambda - 2\pi \delta f \delta_{\mu\nu})^2 + \cdots + \frac{1}{2} (\partial_\mu \theta_-)^2 + 2\lambda \cos 3\theta_- \tag{4}$$

where $\theta_\pm = \theta_a \pm \theta_b$.

Obviously, the $\theta_-$ sector is massive (namely, $\theta_a$ and $\theta_b$ are locked together) and can be integrated out. Assuming $\lambda > 0$, then $\theta_- = \pi$. Setting $\psi_a = e^{i\theta_a} \sim \psi_a - \sim \psi_b$ in Eqn.2 leads to Eqn.3 with $u = 2\gamma_0$, so the discussions on Ising limit case following Eqn.3 also apply. In the present boson problem with possible ring exchange interactions in Eqn.1 which stabilizes the VBS state at $f = 1/2$, this corresponds to a VBS supersolid (VB-SS) state intruding between the commensurate VBS (C-VBS) state at $f = 1/2$ and the incommensurate VBS (IC-VBS) state at $1/2 + \delta f$ as shown in Fig.1b. In this IC-VBS state, $\delta f$ valence bonds shown in Fig.1a is slightly stronger than the others. In the VB-SS state, $< \psi_a > - < \psi_b > = 0$, but $< \psi_a^3 \psi_a > - < \psi_b^3 \psi_b > = - < \psi_a^3 \psi_b > - 0$, so there is a VBS order $K_{AB} = \cos(Q \cdot \vec{r} + \theta_-)$ which is the same as the C-VBS, the superfluid density $\rho_s \sim \delta f$. Again, the first transition is in the $z = 2, \nu = 1/2, \eta = 0$ universality class, while the second is 1st order. The nature of the transition from the VB-SS to the SF where $< \psi_a > - < \psi_b > = 0$ and $< \psi_b^3 > = 0$ inside the window driven by the quantum fluctuation $r$ in the Fig.2b will be studied in [13].

6. Square lattice. As said below Eqn.2 with correspondingly defined $\psi_{a/b}$ in a square lattice, up to the quartic level, Eqn.2 is the same as that in the square lattice derived in [13]. So in the Ising limit, Fig.2b remains the same as Fig.1b. However, in the Easy-plane limit, as shown in [13], the lowest order term coupling the two phases $\theta_{a/b} = C_{sq} = \lambda \cos 4\theta$. If $\lambda$ is positive (negative), the VBS is Columnar dimer (plaquette) pattern. So the
C3 term in Eqn.11 need to be replaced by Csq. Because Csq is irrelevant near the QCP, the transition from the SF to the VBS could be a 2nd order transition through the deconfined QCP [19] as shown in Fig.2c. We expect that the SF to the VB-SS transition could also be 2nd order through a novel deconfined quantum critical point. (b) and (c) are drawn only above half filling. The first order transition in (b) is a strong one.

7. Implication on Quantum Monte-Carlo (QMC) simulations. QMC simulations of hard core bosons on square lattice with V1 and V2 interactions find a stable striped ($\pi,0$) and $(0,\pi)$ SS (Fig.3b) [9]. A stable ($\pi,\pi$) SS can be realized in soft core boson case. But the nature of the CDW to supersolid transition has never been addressed. Our results show that the CDW to the SS transition must be in the same universality class of Mott to superfluid transition with exact exponents $z = 2, \nu = 1/2, \eta = 0$ with logarithmic corrections. It is important to (1) confirm this prediction by finite size scaling through the QMC simulations in square lattice for ($0,\pi$) and ($\pi,0$) supersolid in hard core case (Fig.3b) and ($\pi,\pi$) supersolid in the soft core case (2) do similar things in honeycomb lattice to confirm Fig.1. (3) To Eqb.11 with $U = \infty, V_1 > 0$, adding ring exchange term $-K_s \sum_{ijk} (b_i^\dagger b_j^\dagger b_k + h.c.)$ [9] where $i,j,k,l$ label 4 corners of a square in the square lattice and $-K_h \sum_{ijklmn} (b_i^\dagger b_j^\dagger b_k^\dagger b_l b_i b_j b_k b_l + h.c.)$ where $i,j,k,l,m,n$ label 6 corners of a hexagon in the honeycomb lattice to stabilize the C-VBS state at half filling ($K_s, K_h > 0$ are free of sign problem in QMC ), then confirm the prediction on C-VBS to VB-SS transition in Fig.2c and Fig.1c. The second transition (CDW-SS to IC-CDW in Fig. 1b or 2b and the VB-SS to IC-VBS in Fig 1c or Fig.2c ) is hard to be tested in QMC, because some very long range interactions are needed to stabilize the IC-CDW or the IC-VBS state. They are first order transition anyway.

In fact, one of the predictions in this letter on the scaling of the superfluid density $\rho_s \sim |\rho - 1/2|$ was already found in the striped $(\pi,0)$ solid to striped supersolid transition by QMC in Sec.V-B [7]. In fact, as shown in section 4, there should be logarithmic correction to the scaling of $\rho_s$, it remains a challenge to detect the logarithmic correction in QMC. Of course, the superfluid density is anisotropic $\rho_s^x > \rho_s^y$ in the $(\pi,0)$ solid, but they scale in the same way with different coefficients [7]. Although the authors in [7] suggested it is a 2nd order transition, they did not address the universality class of the transition.

8. Summary We studied some phases and phase transitions in an extended boson Hubbard model near half filling on bipartite lattices such as honeycomb and square lattice. We identified boson density and boson kinetic energy operators to characterize symmetry breaking patterns in the insulating states and supersolid states. We found that in the insulating side, the transition at zero temperature driven by the chemical potential must be a C-CDW (or C-VBS) at half filling to a narrow window of CBW (or VB-) supersolid, then to a IC-CDW (or IC-VBS) transition in the Ising (easy-plane) limit. The valence bond supersolid is a new kind of supersolid first proposed in this letter. The first transition is in the same universality class as that from a Mott insulator to a superfluid driven by a chemical potential, therefore have exact exponents $z = 2, \nu = 1/2, \eta = 0$ with logarithmic corrections. The second is a 1st order transition. The results achieved in this letter could guide QMC simulations to search for all these phases and confirm the universality class of the transitions. These transitions could be easily realized in near future atomic experiments in optical lattices.
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