Bose-Einstein supersolid phase for a novel type of momentum dependent interaction

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A novel class of non-local interactions between bosons is found to favor a crystalline Bose-Einstein condensation ground state. By using both low energy effective field theory and variational wavefunction method, we compare this state not only with the homogeneous superfluid, but has been done previously, but also with the normal (non-superfluid) crystal phase and obtain the phase diagram. The key characters are: the interaction potential displays a negative minimum at finite momentum which determines the wavevector of this supersolid phase; and the wavelength corresponding to the momentum minimum needs to be greater than the mean inter-boson distance.

Since Penrose and Onsager’s first discussion on existence of “supersolid”, namely a phase with co-existence of superfluid and crystalline order, both experimental and theoretical attempts have been made for decades in the search of this novel phase. Recently reported observation of “supersolid” phase in He-4 systems reinvigorated this fundamental interest. Nevertheless, some subsequent experimental evidences as well as various proposed microscopic mechanisms remain controversial.

Progress on the physics of cold atoms and molecules opens a new possibility to study the “supersolid” phase thanks to clean and controlled experimental systems. One of the most fascinating facts is the unprecedented tunability of the interaction potentials due to internal degrees of freedom of atoms and molecules, which allows one to address a theoretical question, namely what interaction potentials can support the supersolid phase in continuous space. Recent experimental progress on dipolar quantum gases allows to explore new physics of quantum many body systems with non-local interactions. It is well established that non-local interaction potentials stabilize the supersolid phase on lattice. The possibility of finding a Bose-Einstein supersolid phase was also put forward for several continuum model systems such as dipolar quantum gases, atom-molecule mixture gases and Rydberg atom gases. Recently, Henkel et al. found that the Fourier transform of an isotropically repulsive van der Waals interaction potential with a “softened” core has a partial attraction in momentum space, which gives rise to a transition from a homogeneous Bose-Einstein condensate to a supersolid phase due to roton instability. However, whether the supersolid phase they found is stable against fluctuations and how it should compare with the non-superfluid (normal) IC phase they found is stable against fluctuations due to roton instability. However, whether the supersolid phase exists or not, it can be considered as a transition to a supersolid phase.

Next, we shall study as a concrete example the “softened” dipolar interaction recently proposed for Rydberg atomic gases. We will establish the ground state in the sense of variational principle and find a first order phase transition from the uniform superfluid phase to the triangular crystalline phase. Finally, we shall compare the energies of BES and IC phases of the same lattice configurations, and find a regime in which the triangular-lattice BES is stable and has lower energy than both USF and (normal) IC. The result is summarized in Fig. 1.

Hamiltonian and heuristic. To explore the physics of the BES phase, we start with the continuum Hamiltonian of two dimensional interacting bosons

\[ H = \int d^2 \bar{r} \hat{\psi}^\dagger(\bar{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \hat{\psi}(\bar{r}) + \frac{1}{2} \int d^2 \bar{r}_1 d^2 \bar{r}_2 \hat{\psi}^\dagger(\bar{r}_1) \hat{\psi}^\dagger(\bar{r}_2) V(\bar{r}_1 - \bar{r}_2) \hat{\psi}(\bar{r}_2) \hat{\psi}(\bar{r}_1), \]

where the first term of \( H \) corresponds to the kinetic energy, and the second the two-body interaction energy.

It is commonly accepted that the ground state for such a continuous bosonic system should be USF at the kinetic energy dominating regime. The USF phase is described by a coherent state \( |\text{USF}\rangle = \exp\left[ \int d^2x \sqrt{n} e^{i\phi} \hat{\psi}^\dagger(x) \right] |\Omega\rangle \) where \( n \) is the mean particle density, \( \phi \) a constant phase, and \( |\Omega\rangle \) the vacuum state with no particle. The energy of this state is given by \( E_{\text{USF}} = N \frac{\hbar^2}{2m} \langle k | = 0, \rangle \), where \( N \) is the mean particle number and \( U(k) \) is Fourier transform of the interaction potential. We first analyze the
instability of the USF phase. This can be performed using an effective field theory approach [15, 16]. The real time action of this bosonic system is \( S[\psi, \psi^\dagger] = \int d^2x dt \{ i\hbar \partial_t \psi - \mathcal{H}[\psi, \psi^\dagger] \} \). Fluctuations on top of the uniform superfluid state are considered by writing the boson field \( \psi(x, t) = [\rho_0 + \delta \rho(x,t)]e^{i\phi(x,t)} \), assuming \( \delta \rho \) and \( |\nabla \phi| \) are small. The quasiparticle spectrum is readily derived after integrating out the \( \delta \rho \) field: \( \epsilon(k) = \sqrt{\frac{k^2 \hbar^2}{2m} + nU(k)} \). For a potential that has a negative minimum at a finite momentum, this spectrum at that momentum drops, eventually hits zero and becomes imaginary when increasing the density \( n \). That suggests that the assumed USF (coherent) state is unstable towards possible crystalline order.

To show the BES phase arises, we first give a heuristic argument by considering a simple stripe BES state \( |\text{BES}\rangle = \exp\left( i\sqrt{N}(\frac{\mathbf{Q}}{2}\mathbf{b}_0 + \frac{\mathbf{Q}}{2}\mathbf{b}_0^\dagger)\right)|\Omega\rangle \), where \( \mathbf{Q} = [Q, 0] \), and \( \mathbf{Q} \) the minimum point of \( U(k) \). The energy of this state is given by \( E_{\text{BES}} = N \left( \frac{k^2 \hbar^2}{2m} + \frac{1}{2}nU(\mathbf{Q}) \right) + E_{\text{USF}} \). When the term \( \frac{k^2 \hbar^2}{2m} + \frac{1}{2}nU(\mathbf{Q}) \) is negative, namely the interaction energy dominates over the kinetic energy, the stripe BES state has lower energy than the USF state. (We also go beyond the mean field state and compare with the two component fragmented state \( |f\rangle = \sum_{l=-N/2}^{l=N/2} \alpha_l \left( \frac{\mathbf{Q}}{2}\mathbf{b}_l + \frac{\mathbf{Q}}{2}\mathbf{b}_l^\dagger \right) \right)|\Omega\rangle \), where \( \{\alpha_l\} \) are variational parameters [17], and the coherent stripe BES state is found to have the lowest energy.) We thus conclude the BES state arises from the competition of kinetic energy and interaction energy.

To be concrete, we further apply the two-particle interaction of a step-like form \( V(r) = \frac{\tilde{D}}{r_0^2} \) if \( r < r_d \); \( V(r) = \frac{\tilde{D}}{r} \) otherwise. The form of this potential is an approximation to the interaction between polarized Rydberg atoms proposed in Ref. [17]. Two dimensionless parameters of this system are \( \tilde{n} \equiv n \times r_0^2 \) and \( r_d \equiv 2mD^2n^{-1/2} \). \( \tilde{n} \) characterizes the relation between \( r_0 \) and the inter-particle distance, and \( r_d \) characterizes the strength of interaction. A phase transition from USF to IC has been found when varying \( r_d \) at the regime of \( \tilde{n} \approx 0.9 \) [14]. The IC (single particle per site) phase is described in a second quantization form by \( |\Psi_{\text{IC}}\rangle = \prod_{\mathbf{k}} \mathcal{R}_\mathbf{k} c_{\mathbf{k}}^\dagger |0\rangle \), where \( \mathcal{R}_\mathbf{k} \) is the direct lattice vector at site \( i \), and the single particle wavefunction corresponding to \( c_{\mathbf{k}}^\dagger \) is the Wannier function \( \phi_{\mathbf{k}}(\mathbf{r}) \).

The Fourier transform of this step-like interaction is shown in FIG. 2(a). It is straightforward to obtain the excitation spectrum, which is shown in FIG. 2(b). It can be seen that the spectrum displays instability. The origin of this effect is that the Fourier transform of the interaction, \( U(k) \), has a negative minimum at a finite momentum. Now the question is to find the stable variational minimum in the coherent state space. With \( |G\rangle = \exp(\int d^2x \phi(x)\hat{\phi}^\dagger(x)|\Omega\rangle \) (so that \( \hat{\phi}(x)|G\rangle = \phi(x)|G\rangle \)), the energy of this state is readily given by:

\[
E[\phi, \phi^*] = \int d^2r \frac{\hbar^2}{2m} |\nabla \phi|^2 + \frac{1}{2} \int d^2r_1 d^2r_2 V(\mathbf{r}_1 - \mathbf{r}_2) \phi(\mathbf{r}_1)^2 |\phi(\mathbf{r}_2)|^2 ,
\]

where \( V(\mathbf{r}) \) is the interaction potential.

**Variational analysis.** We first check whether the system favors an extended or localized state. This purpose is fulfilled by applying the Gaussian ansatz which means \( \phi(\mathbf{r}) = \frac{\sqrt{N}}{\sqrt{2\pi}^{d/2}} e^{-\frac{r^2}{2\sigma^2}} \). The total energy of this system is given by \( E_t = E_k + E_{\text{U}ip} \), where the kinetic energy \( E_k = \int d^2r \frac{\hbar^2}{2m} |\nabla \phi|^2 \), the interaction energy \( E_{\text{U}ip} = \int d^2r \frac{\hbar^2}{2m} |\nabla \phi|^2 \), and the effective potential energy \( E_{\text{E}ip} = \int d^2r \frac{\hbar^2}{2m} |\nabla \phi|^2 \).
We found that as long as \( \int d^2r \mathcal{V}(\vec{r}) > 0 \), \( \sigma \to \infty \) maximizes the energy, implying the system favors an extended state in space. Since for \( r_d > 0 \) \( \int d^2r \mathcal{V}(\vec{r}) > 0 \), we conclude that the system favors an extended state when \( r_d \) is positive.

Up to this point, what we know about this system is that it favors an extended state which is not necessarily uniform superfluidity. Having argued heuristically above that a momentum dependent interaction may favor a finite momentum BEC, it is natural to compare the energy of a new, non-uniform coherent state which has discrete lattice symmetries. Thus, we can write the condensate wavefunction in such a form \( \phi(\vec{r}) = |\psi(\vec{r})| = \sqrt{N} \sum_{\mathbf{K}} \phi_{\mathbf{K}} e^{i \mathbf{K} \cdot \vec{r}} \) with \( \mathbf{K} = p \mathbf{G}_1 + q \mathbf{G}_2 \), where \( \mathbf{G}_1 \) and \( \mathbf{G}_2 \) are two primitive vectors spanning the two dimensional reciprocal lattice. The corresponding ground state is \( |G\rangle = \exp \left( \sum_{\mathbf{K}} \sqrt{N} \phi_{\mathbf{K}} b_{\mathbf{K}}^\dagger \right) |\Omega\rangle \). The order parameter that characterizes the phase transition from uniform superfluidity to BE supersolidity is an occupation fraction at some finite momentum \( K \), \( |\phi_{\mathbf{K}}|^2 = \frac{1}{N} \langle b_{\mathbf{K}} b_{\mathbf{K}}^\dagger \rangle \).

In this assumed ground state subspace, the energy per particle is given by:

\[
E[\phi_K, \phi_{\mathbf{K}}] = \sum_{\mathbf{K}} \frac{\hbar^2 K^2}{2m} \phi_{\mathbf{K}}^\dagger \phi_{\mathbf{K}} + \frac{1}{\pi} \sum_{q, K_1, K_2} U(q) \phi_{K_1+q}^\dagger \phi_{K_2-q} \phi_{K_2} \phi_{K_1},
\]

Now, the problem reduces to minimizing this energy functional with such a constraint \( \sum_{\mathbf{K}} |\phi_{\mathbf{K}}|^2 = 1 \), which is equivalent to the enforcement of conservation of the total particle number. By \( \delta(E - \mu \sum_{\mathbf{K}} \phi_{\mathbf{K}}^\dagger \phi_{\mathbf{K}})/\delta(\phi_{\mathbf{K}}) = 0 \), we obtain

\[
\mu \phi_{\mathbf{K}} = \frac{\hbar^2 K^2}{2m} \phi_{\mathbf{K}} + \frac{1}{\pi} \sum_{K', q} U(q) \phi_{K' + q}^\dagger \phi_{K'} \phi_{K+q},
\]

where \( \mu \) is the chemical potential.

We compute the energies for three different configurations — stripe, square and triangle lattices — and found that the triangular lattice is the most energetically favored. The optimal lattice constant \( a_{\text{BES}} \) is found to be slightly larger than \( 2\pi/Q_{\text{min}} \) where \( U(Q_{\text{min}}) \) corresponds to the negative minimum of the potential. For the particular step-like interaction, \( Q_{\text{min}} \) is related to \( r_0 \) by \( Q_{\text{min}} \approx \frac{3 \pi}{2} \approx \frac{3 \pi}{\sqrt{2}} \). The transition between the uniform superfluid and the supersolid lattice is of first order as shown in FIG. 2.

Dynamic stability of the Bose-Einstein supersolid phase. To study the stability of the BES phase, we further explore the fluctuations on top of the ground state. In the presence of BES phase, we can get the effective field theory for the density and phase fluctuations \( \delta \rho(x, t) \) and \( \varphi(x, t) \), respectively, writing \( \psi(x, t) = |\rho_0(x) + \delta \rho(x, t)|^{1/2} e^{i \varphi(x, t)} \), where \( \rho_0(x) = |\phi(x)|^2 \). The effective action for \( \delta \rho \) and \( \varphi \) to quadratic order is

\[
S_{\text{eff}}[\delta \rho, \varphi] = \int dt \int d^2x \mathcal{L}(x, t),
\]

\[
\mathcal{L} = -\frac{\hbar^2}{2m} \frac{\delta \rho_{\mathbf{K}}}{\sqrt{\rho_0}}^2 - \frac{1}{8} \hbar^2 \left( \frac{\delta \rho}{\sqrt{\rho_0}} \right)^2 - \frac{1}{2} \rho_0 \hbar^2 \left( \frac{\delta \varphi}{\sqrt{\rho_0}} \right)^2
\]

where \( \rho_0(x) \) is the modulus square of the condensate wavefunction.

Since the effective theory possesses only discrete translational symmetries, a Brillouin zone and its reciprocal lattice vectors can be defined. Let \( \eta(x) \equiv \frac{\delta \rho(x)}{\sqrt{\rho_0}} \). The effective action in the momentum space is

\[
S_{\text{eff}}[\eta, \varphi] = \int dt \int \sum_{k \in R} \sum_{K_1, K_2} \left[ A_K \eta_{K_1, K_2}(k) \eta_{K_1+k} \delta \varphi_{K_2+k}^* \right]
\]

\[
+ B_K \eta_{K_1, K_2}(k) \eta_{K_1+k} \varphi_{K_2+k} + C_K \eta_{K_1, K_2}(k) \varphi_{K_1+k} \varphi_{K_2+k}^* + \text{c.c.},
\]

with

\[
A_K \eta_{K_1, K_2}(k) = -\alpha_{-K_1, K_2},
\]

\[
B_K \eta_{K_1, K_2}(k) = -\frac{1}{8} \hbar^2 (K_1 + k)^2 \delta \varphi_{K_1, K_2}
\]

\[
- \frac{1}{2} \sum_K \alpha_K \alpha_{K_1-K_2-K} U(k + K_2 - K),
\]

\[
C_K \eta_{K_1, K_2}(k) = \frac{1}{2} \sum_K \hbar^2 |(K_1 + k) \cdot (-K_2 - k)| \alpha_K \alpha_{K_2-K_1-K}
\]

where \( K_1, K_2 \) are reciprocal lattice vectors and \( \alpha_K \) is the Fourier component of \( \sqrt{\rho_0(x)} \). The first Brillouin zone is divided into ‘R’ (right) and ‘L’ (left) subzones according to time reversal; the summation \( k \in R \) in Eq. 9 means summing over the ‘R’ subzone. The above effective theory is quadratic in fields. Formally, the action can be written in a block diagonal form as:

\[
S_{\text{eff}} = \sum_{k \in R} \left[ \eta^T \eta(k) \right] G_k^{-1} \left[ \eta(k) \right],
\]

where the crystal momentum \( k \) is a good quantum number, and \( \eta(k) \) and \( \varphi(k) \) correspond to column vectors formed by \( \{\eta_{K, k} \} \) and \( \{\varphi_{K, k} \} \) with \( K \) running over \( p \mathbf{G}_1 + q \mathbf{G}_2 \). The energy spectrum is determined by the poles of \( G_k \), i.e., \( \det(G_k^{-1}) = 0 \). FIG. 3 shows typical
results we obtained, which indicate the stability of the BES phase. However, for sufficiently large \( r_b \), the spectrum becomes imaginary near \( \mathbf{k} = \mathbf{0} \) (crystal momentum) point indicating instability of the BES state. The stable regime of the BES state are shown in the phase diagram FIG. 1.

Variationally compared with insulating crystal. We further estimate the energy of the IC state. The IC state is described by \( |\Psi_{IC}\rangle = \prod_{\vec{R}_i} c_{\vec{R}_i}^\dagger |0\rangle \) where the single particle wavefunction corresponding to the creation operator \( c_{\vec{R}_i}^\dagger \) is the Wannier function \( \phi_{\vec{R}_i}(\vec{r}) \). Here we consider the case where each localized wave function contains exactly one boson, forming a triangular lattice. The lattice constant \( a_c \) is thus determined by the density \( a_c = [2/(\sqrt{3} n)]^{1/2} \), which is different from the lattice constant of BES, \( a_{BES} \), determined by the minimum point of \( U(k) \).

In the phase diagram (FIG. 1), the BES is stable and is the most energy-favored in the ‘yellow shaded’ regime. The lower boundary is determined by comparing the energy of BES state and \( E_{IC}(\sigma = 0.3a_c) \) while the right boundary is computed from the instability of the BES spectrum. In the ‘unstable’ regime, the proposed BES state has lower energy than the IC state but is not stable against quantum fluctuations.

In conclusion, we studied a bosonic system with two-body interaction potentials which display a negative minimum at a finite momentum and found a stable supersolid phase arising from Bose-Einstein condensation at finite momenta. The stability of this novel supersolid phase is checked against quantum fluctuation. A unique feature of the BES state is that it breaks both \( U(1) \) and translational symmetry with a single order parameter, namely, the superfluid order parameter \( \langle \psi(\vec{r}) \rangle \) is not only finite but also spatially modulated. The physical interpretation is that particles are not localized in space but condensed to a single, common wavefunction which is modulated like a solid. This is conceptually different from one of widely considered supersolid pictures of He-4 [1,4] in which supersolidity is a mixture of two orderings: atoms form charge-density-wave order (a crystal structure) and in the same time vacancies or interstitials undergo usual (zero-momentum) Bose-Einstein condensation. For the conventional superfluid phase originated from zero-momentum BEC, there exists long range phase coherence but the phase correlation function is homogeneous, not modulated, in space. In contrast, for the IC (insulating crystal) phase, particles are localized in space to each lattice site, so there is no long range phase coherence. Therefore, as prediction for cold gas experiments, a signature of the new BES phase is the modulated phase coherence. This new state also opens fundamental questions for future studies, for example, how the supercurrent is affected by the simultaneous presence of crystalline ordering, and topological configurations such as a vortex coupled to a crystal defect.

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Note Added. Near the completion of this paper, a related, independent study appeared [20], which discovered by exact numerical algorithms for a similar model system a supersolid phase to occur in the same parameter regime.

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