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

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A class of nonlocal interactions between bosons is found to favor a crystalline Bose-Einstein condensation ground state. By using both low-energy effective field theory and a variational wave function method, we compare this state not only with the homogeneous superfluid, as has been done previously, but also with the normal (nonsuperfluid) crystalline phase and obtain the phase diagram. The key characters are (1) the interaction potential displays a negative minimum at finite momentum, which determines the wave vector of this supersolid phase, and (2) the wavelength corresponding to the momentum minimum needs to be greater than the mean interboson distance.

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Since Penrose and Onsager's first discussion [1] on the existence of supersolids, namely, a phase with coexistence of superfluid and crystalline order, both experimental [2] and theoretical [3] attempts have been made for decades in search of this phase. Recently reported observations of a supersolid phase in ⁴He systems [4] revitalized this fundamental interest. Nevertheless, some subsequent experimental evidence as well as various proposed microscopic mechanisms [5] 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 because of internal degrees of freedom of atoms and molecules [6,7], 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 us to explore new physics of quantum many-body systems with nonlocal interactions [8]. It is well established that nonlocal interaction potentials stabilize the supersolid phase on the lattice [9]. The possibility of finding a Bose-Einstein supersolid phase [10] was also put forward for several continuum model systems such as dipolar quantum gases [11], atom-molecule mixture gases [12], and Rydberg atom gases [7,13]. Recently, Henkel et al. [13] 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 (BEC) to a supersolid phase because of roton instability. However, whether the supersolid phase they found is stable against fluctuations and how it should compare with the nonsuperfluid (normal) crystal phase has not been studied. Recent work on dipolar gases [14] showed that the dipolar dominating interaction does not support a supersolid phase in the phase diagram between the uniform superfluid and the normal crystal phase, where this phase had been speculated to exist.

In this Rapid Communication, we show that interaction potentials, which display a minimum of negative value at a finite momentum, lead to a modulating superfluid order, namely, a Bose-Einstein supersolid (BES) phase. We perform effective field theory analysis and variational calculation to determine not only the phase boundary between the uniform superfluid (USF) phase and BES, which has been previously analyzed by roton instability for dipolar [10,11] or van der Waals interaction [13], but also the phase boundary between BES and the normal (nonsuperfluid) insulating crystal (IC) phase. We shall begin with a heuristic argument to show how a stripe BES phase should arise from the competition between kinetic and interaction energy in the regime of roton instability. Next, we shall study as a concrete example the softened dipolar interaction recently proposed for Rydberg atomic gases [7]. A similar potential is also proposed in Ref. [13]. 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 BES 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.

To explore the physics of the BES phase, we start with the continuum Hamiltonian of two-dimensional interacting bosons:

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

where the first term of H corresponds to the kinetic energy and the second to 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 $|\text{USF}\rangle = \exp[\int d^2x \sqrt{n}e^{i\phi_0}\hat{\psi}^{\dagger}(x)]|\Omega\rangle$, where *n* is the mean particle density, ϕ_0 a constant phase, and $|\Omega\rangle$ is the vacuum state with no particle. The energy of this state is given by $E_{\text{USF}} = (N/2)nU(\mathbf{k} = \mathbf{0})$, where *N* is the mean particle number and $U(\mathbf{k})$ 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 $S[\bar{\psi}, \psi] = \int d^2x \, dt \{i\hbar\bar{\psi}\partial_t\psi - \mathcal{H}[\bar{\psi}, \psi]\}$. Fluctuations on

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FIG. 1. (Color online) The phase diagram of bosons with steplike interaction. USF, IC, and BES phases are separated by solid lines with crosses showing the data points from variational calculation. Analysis of the collective excitation spectrum shows the instability of USF at the red dotted line and that of BES at the dark blue dash-dotted line. At low density, the USF phase and IC phase exist, while at high density, a stable BES phase is found in the yellow shaded regime. When $\tilde{n} \gtrsim 1$, the IC state is not stable (see text).

top of the uniform superfluid state are considered by writing the boson field $\psi(x,t) = [\rho_0 + \delta\rho]^{1/2} e^{i\phi}$, assuming $\delta\rho$ and $|\nabla\phi|$ are small. The quasiparticle spectrum is readily derived after integrating out the $\delta\rho$ field:

$$\epsilon(\mathbf{k}) = \sqrt{\frac{\hbar^2 \mathbf{k}^2}{2m}} \left[\frac{\hbar^2 \mathbf{k}^2}{2m} + 2nU(\mathbf{k}) \right].$$

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 toward possible crystalline order.

To show the BES phase arises, we first give a heuristic argument by considering a simple stripe BES state $|\text{BES}\rangle = \exp\{\sqrt{N}[(\sqrt{2}/2)b_{\mathbf{Q}/2}^{\dagger} + (\sqrt{2}/2)b_{-\mathbf{Q}/2}^{\dagger}]\}|\Omega\rangle$, where $\mathbf{Q} = [Q,0]$ and \mathbf{Q} is the minimum point of $U(\mathbf{k})$. The energy of this state is given by $E_{\text{sBES}} = N[(\hbar^2 Q^2/8m) + (1/4)nU(\mathbf{Q})] + E_{\text{USF}}$. When the term $(\hbar^2 Q^2/8m) + (1/4)nU(\mathbf{Q})$ 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

$$|f\rangle = \sum_{l=-N/2}^{l=N/2} \alpha_l \frac{(b_{\mathbf{Q}/2}^{\dagger})^{\frac{N}{2}+l}(b_{-\mathbf{Q}/2}^{\dagger})^{\frac{N}{2}-l}}{\sqrt{(\frac{N}{2}+l)!}\sqrt{(\frac{N}{2}-l)!}} |\Omega\rangle,$$

where $\{\alpha_l\}$ are variational parameters [17] and the coherent stripe BES state is found to have the lowest energy.) We thus conclude that 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 steplike form $V(\vec{r}) = D/r_0^3$ if $r < r_0$; $V(r) = D/r^3$ otherwise. The form of this potential is an approximation to the interaction between polarized Rydberg atoms proposed in Ref. [7]. Two dimensionless parameters of this system are $\tilde{n} \equiv n \times r_0^2$ and $r_d \equiv 2mDn^{1/2}/\hbar^2$; \tilde{n} characterizes the relation between r_0 and the interparticle distance, and r_d characterizes the strength of interaction. A phase transition from USF to IC





FIG. 2. (Color online) (a) Fourier transform of the steplike twobody interaction. (b) Bogoliubov quasiparticle spectrum for a USF state. The plot shows the real part of the spectrum with $\tilde{n} = 1$. The solid line corresponds to $r_d = 5$, the dashed line to $r_d = 15$, and the dash-dotted line to $r_d = 23$. (bottom) Phase transition from the USF to the triangular crystalline BES phase. $|\phi_{\mathbf{K}}|^2 \equiv 1/N \langle b_{\mathbf{K}}^{\dagger} b_{\mathbf{K}} \rangle$ is the occupation fraction of the lowest finite momentum.

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 $|\Psi_{\text{IC}}\rangle = \prod_{\vec{R}_i} c^{\dagger}_{\vec{R}_i} |0\rangle$, where \vec{R}_i is the direct lattice vector at site *i*, and the single particle wave function corresponding to $c^{\dagger}_{\vec{R}_i}$ is the Wannier function $\phi_{\vec{R}_i}(\vec{r})$.

The Fourier transform of this steplike 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, $U(\mathbf{k})$, has a negative minimum at a finite momentum. Now the question is to find the stable variational minimum in the coherent state space. With $|G\rangle = \exp[\int d^2 \mathbf{x} \phi(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{x})] |\Omega\rangle$ [so that $\hat{\psi}(\mathbf{x}) |G\rangle = \phi(\mathbf{x}) |G\rangle$], the energy of this state is readily given by

$$E = \int d\mathbf{r} \frac{\hbar^2}{2m} |\vec{\nabla}\phi|^2 + \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) |\phi(\mathbf{r}_1)|^2 |\phi(\mathbf{r}_2)|^2,$$
(2)

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

. 2

We first check whether the system favors an extended or localized state. This purpose is fulfilled by applying the Gaussian ansatz, which means $\phi(\vec{r}) = (\sqrt{N}/\sqrt{\pi})\sigma e^{-(|\vec{r}|^2/2\sigma^2)}$. The total energy of this system is given by $E_t = E_k + E_{dip}$, where the kinetic energy $E_k = N(\hbar^2/2m\sigma^2)$ and the interaction energy $E_{dip} = N^2(1/2\pi^2)(D/r_0^3)g(r_0/\sigma)$. Here g(x) is approximately $\pi^2(1 - e^{-2x^2})$. The energy per particle is $(\hbar^2/2m\sigma^2) + (ND/2\pi^2r_0^3)g(r_0\sigma)$. In the thermodynamic limit $N \to \infty$, interaction dominates, and $E(\sigma) = (ND/2\pi^2r_0^3)g(r_0/\sigma)$. We found that as long as $\int d^2\vec{r}V(\vec{r}) > 0$, $\sigma \to \infty$ minimizes the energy, implying that the system favors an extended state in space. Since for $r_d > 0$, $\int d^2\vec{r}V(\vec{r}) > 0$, we conclude that the system favors an extended state when r_d is positive.

Up to this point, we have learned that this system favors an extended state which is not necessarily a uniform superfluid. Having argued heuristically that a momentum-dependent interaction may favor a BES state, it is natural to compare the energy of a nonuniform coherent state which has discrete lattice symmetries. Thus we can write the condensate wave function in such a form: $\phi(\vec{r}) = \langle \psi(\vec{r}) \rangle = \sqrt{n} \sum_{\mathbf{K}} \phi_{\mathbf{K}} e^{i\mathbf{K}\cdot\vec{r}}$, 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 $|G\rangle = \exp(\sum_{\mathbf{K}} \sqrt{N}\phi_{\mathbf{K}} b_{\mathbf{K}}^{\dagger})|\Omega\rangle$. The order parameter that characterizes the phase transition from USF to BES is an occupation fraction at some finite momentum K, $|\phi_{\mathbf{K}}|^2 = 1/N \langle b_{\mathbf{K}}^{\dagger} b_{\mathbf{K}} \rangle$. In this assumed ground state subspace, the energy per particle is given by

$$E = \sum_{\mathbf{K}} \frac{\hbar^2 K^2}{2m} \phi_{\mathbf{K}}^* \phi_{\mathbf{K}} + \frac{n}{2} \sum_{\mathbf{K}_1, \mathbf{K}_2, \mathbf{q}} U(\mathbf{q}) \phi_{\mathbf{K}_1 + \mathbf{q}}^* \phi_{\mathbf{K}_2 - \mathbf{q}}^* \phi_{\mathbf{K}_2} \phi_{\mathbf{K}_1}.$$
(3)

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 $\delta(E - \mu \sum_{\mathbf{K}} \phi_{\mathbf{K}}^* \phi_{\mathbf{K}}) / (\delta \phi_{\mathbf{K}}^*) = 0$, we obtain

$$\mu\phi_{\mathbf{K}} = \frac{\hbar^2 K^2}{2m} \phi_{\mathbf{K}} + n \sum_{\mathbf{K}',\mathbf{q}} V(\mathbf{q}) \phi^*_{\mathbf{K}'+\mathbf{q}} \phi_{\mathbf{K}'} \phi_{\mathbf{K}+\mathbf{q}} , \qquad (4)$$

where μ is the chemical potential.

We computed 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_{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 steplike interaction, Q_{min} is related to r_0 by $Q_{\text{min}} \approx 3.9/r_0 \sim \pi/r_0$. The transition between USF and BES is of first order, as shown in Fig. 2.

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

$$S_{\rm eff}[\delta\rho,\varphi] = \int dt \int d^2 \mathbf{x} \mathscr{L}(\mathbf{x},t) ,$$
$$\mathscr{L} = -\hbar \delta\rho \partial_t \varphi - \frac{1}{8} \hbar^2 \left(\vec{\nabla} \frac{\delta\rho}{\sqrt{\rho_0}}\right)^2 - \frac{1}{2} \rho_0 \hbar^2 (\vec{\nabla}\varphi)^2 \quad (5)$$
$$- \frac{1}{2} \int d^2 \mathbf{x}' V(\mathbf{x} - \mathbf{x}') \delta\rho(\mathbf{x},t) \delta\rho(\mathbf{x}',t) ,$$

¹Another collective mode of the BES phase is lattice vibrations. All low-energy fluctuations shall be studied together systematically in the future. where $\rho_0(\mathbf{x})$ is the modulus square of the condensate wave function.

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

$$S_{\rm eff} = \int dt \sum_{\mathbf{k}\in\mathbf{R}} \sum_{\mathbf{K}_{1},\mathbf{K}_{2}} [A_{\mathbf{K}_{1}\mathbf{K}_{2}}(\mathbf{k})\eta_{\mathbf{K}_{1}+\mathbf{k}}(\partial_{t}\varphi_{\mathbf{K}_{2}+\mathbf{k}}^{*}) + B_{\mathbf{K}_{1}\mathbf{K}_{2}}(\mathbf{k})\eta_{\mathbf{K}_{1}+\mathbf{k}}\eta_{\mathbf{K}_{2}+\mathbf{k}}^{*} + C_{\mathbf{K}_{1},\mathbf{K}_{2}}(\mathbf{k})\varphi_{\mathbf{K}_{1}+\mathbf{k}}\varphi_{\mathbf{K}_{2}+\mathbf{k}}^{*}] + \text{c.c.},$$
(6)

 $A_{\mathbf{K}_1\mathbf{K}_2}(\mathbf{k}) = -\alpha_{-\mathbf{K}_1+\mathbf{K}_2},$

with

$$B_{\mathbf{K}_{1}\mathbf{K}_{2}}(\mathbf{k}) = -\frac{1}{8}\hbar^{2}(\mathbf{K}_{1} + \mathbf{k})^{2}\delta_{\mathbf{K}_{1},\mathbf{K}_{2}} - \frac{1}{2}\sum_{\mathbf{K}}\alpha_{\mathbf{K}}\alpha_{\mathbf{K}_{2}-\mathbf{K}_{1}-\mathbf{K}}U(\mathbf{k} + \mathbf{K}_{2} - \mathbf{K}),$$

$$C_{\mathbf{K}_{1}\mathbf{K}_{2}}(\mathbf{k}) = \frac{1}{2}\sum_{\mathbf{K}}\hbar^{2}[(\mathbf{K}_{1} + \mathbf{k}) \cdot (-\mathbf{K}_{2} - \mathbf{k})]\alpha_{\mathbf{K}}\alpha_{\mathbf{K}_{2}-\mathbf{K}_{1}-\mathbf{K}},$$
(7)

where $\mathbf{K}_1, \mathbf{K}_2$ are reciprocal lattice vectors and $\alpha_{\mathbf{K}}$ is the Fourier component of $\sqrt{\rho_0(\mathbf{x})}$. The first Brillouin zone is divided into "R" (right) and "L" (left) subzones according to time reversal; the summation $\mathbf{k} \in R$ in Eq. (6) means summing over the R subzone. The preceding effective theory is quadratic in fields. Formally, the action can be written in a block diagonal form as

$$S_{\text{eff}} = \sum_{\mathbf{k}\in R} [\eta^{\dagger}(\mathbf{k}) \ \varphi^{\dagger}(\mathbf{k})] \mathscr{G}_{\mathbf{k}}^{-1} \begin{bmatrix} \eta(\mathbf{k}) \\ \varphi(\mathbf{k}) \end{bmatrix},$$

with

$$\mathscr{G}_{\mathbf{k}}^{-1} \equiv \begin{bmatrix} \tilde{B}(\mathbf{k})^T + \tilde{B}(\mathbf{k})^* & \tilde{A}(\mathbf{k})^* \partial_t \\ -\tilde{A}(\mathbf{k})^T \partial_t & \tilde{C}(\mathbf{k})^T + \tilde{C}(\mathbf{k})^* \end{bmatrix}, \qquad (8)$$



FIG. 3. (Color online) The excitation spectrum on top of the BES state from the $\Gamma[\equiv (0,0)]$ point to $X[\equiv (\pi/a_{\text{BES}},0)]$, where a_{BES} is the lattice constant of the supersolid lattice. There are branches of spectrum, the lowest three of which are shown.

where the crystal momentum **k** is a good quantum number, and $\eta(\mathbf{k})$ and $\varphi(\mathbf{k})$ correspond to column vectors formed by $\{\eta_{\mathbf{K}+\mathbf{k}}\}\$ and $\{\varphi_{\mathbf{K}+\mathbf{k}}\}\$, with **K** running over $p\mathbf{G}_1 + q\mathbf{G}_2$. The energy spectrum is determined by the poles of $\mathscr{G}_{\mathbf{k}}$, that is, $\det[\mathscr{G}_{\mathbf{k}}^{-1}] = 0$ [15]. Figure 3 shows typical results we obtained which indicate the stability of the BES phase. However, for sufficiently large r_d , the spectrum becomes imaginary near $\mathbf{k} = \mathbf{0}$ (crystal momentum), indicating instability of the BES state. The stable regime of the BES state is shown in the phase diagram of Fig. 1.

We further estimate the energy of the IC state. The IC state is described by $|\Psi_{\rm IC}\rangle = \prod_{\vec{R}_i} c^{\dagger}_{\vec{R}_i} |0\rangle$, where the single-particle wave function corresponding to the creation operator $c_{\vec{R}}^{\dagger}$ 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 $U(\mathbf{k})$. The Wannier function is approximated by a localized Gaussian $\phi_{\vec{R}_i}(\vec{r}) \sim (1/\sqrt{\pi}\sigma) \exp\{-[(\vec{r}-\vec{R}_i)^2/2\sigma^2]\},\$ with σ/a_c ranging from 0 to 0.3, over which the overlap between neighboring Gaussian wave functions can be neglected [18], and the energy is obtained by $E_{\rm IC}(\sigma) = \langle \Psi_{\rm IC} | H | \Psi_{\rm IC} \rangle$. The calculation involves calculating an integral with Monte Carlo methods, which causes some noise of the phase boundary of the IC phase. When $\tilde{n} \gtrsim 1$, minimizing $E_{\rm IC}(\sigma)$ gives $\sigma/a_c \rightarrow 0.3$, indicating that the IC state with the given lattice constant is unstable. We expect insulating crystals with more than one particle per site [19,20] or insulating crystalsupersolid phase separation to exist in the unstable regime.

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 the 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.

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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 BEC at finite momenta. The stability of this supersolid phase is checked against quantum fluctuations. 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 wave function which is modulated like a solid. This is conceptually different from one of the widely considered supersolid pictures of ⁴He [1,4], in which supersolidity is a mixture of two orderings: atoms form charge-density-wave order (a crystal structure) and, at the same time, vacancies or interstitials undergo usual (zero-momentum) BEC. For the conventional superfluid phase originating from zero-momentum BEC, there exists longrange phase coherence, but the phase correlation function is homogeneous, not modulated, in space. In contrast, for the IC phase, particles are localized in space to each lattice site, so there is no long-range phase coherence. Therefore, as predicted for cold gas experiments, a signature of the BES phase is the modulated phase coherence. This 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.

Note added. Recently, a related, independent study appeared [20] that discovered by exact numerical algorithms for a similar model system a supersolid phase occurring in the same parameter regime.

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