Mean-field and stability analysis of two-dimensional flowing soft-core bosons modeling a supersolid

Masaya Kunimi and Yusuke Kato
Department of Basic Science, The University of Tokyo, Tokyo 153-8902, Japan
(Dated: May 1, 2014)

The soft-core boson system is one of the simplest models of supersolids, which have both off-diagonal long-range order (Bose–Einstein condensation) and diagonal long-range order (crystalline order). Although this model has been studied from various points of view, studies of the stability of current-flowing states are lacking. Solving the Gross–Pitaevskii and Bogoliubov equations, we obtain excitation spectra in superfluid, supersolid, and stripe phases. On the basis of the results of the excitation spectra, we present a stability phase diagram that shows the region of the metastable superflow states for each phase.

PACS numbers: 67.80.-s, 03.75.-b

Introduction. A supersolid is a quantum phase that has both superfluidity and solidity. After it was demonstrated in some seminal works\(^1\) that this intriguing state can be realized in quantum solids, much research has been done. Recently, Kim and Chan\(^2\) presented the possibility of a supersolid in solid \(^4\)He. They reported experimental results of non-classical rotational inertia (NCRI) in solid \(^4\)He. While there have been many experimental and theoretical studies made\(^3,4\), there still remains controversy over the origin of NCRI in solid \(^4\)He. Ultra-cold atomic gases have also become a field for the study of supersolids. Many theoretical works support the existence of a supersolid phase in systems with strong long-range interactions such as dipole-dipole\(^5\) or van der Waals interactions\(^6\). Recently, Bose–Einstein condensates (BEC) of \(^{52}\)Cr, \(^{164}\)Dy,\(^7\) and \(^{168}\)Er,\(^8\), which have large magnetic moments, have been realized experimentally. Owing to the high controllability of experimental conditions, cold atomic gases may provide insights into the nature of supersolids.

In the many previous studies, the properties of equilibrium states of supersolids have been investigated. However, dynamical stability of a finite superflow state cannot be obtained by calculating equilibrium states in the absence of a current.\(^9\) We need to investigate the stability of a current-carrying state that has both off-diagonal long-range order (ODLRO) and diagonal long-range order (DLRO).

The stability of condensates can be investigated by calculating the excitation spectra. In many cases, the low-energy excitations determine the critical velocity of superfluids. For example, the Landau critical velocity\(^10\) is determined by the excitation energy, and the critical velocity of a condensate in a moving optical lattice can be calculated from the excitation spectrum.\(^11\) The excitation spectrum can be not only theoretically calculated but also experimentally observed in neutron scattering experiments for \(^4\)He\(^15\) or Bragg spectroscopy of cold atoms.\(^16\) One of the most striking properties of superfluids is the existence of a critical velocity, and determining the critical velocity of a supersolid is an important problem. To determine the supersolid critical velocity, we use a simple continuum model of supersolids that was proposed by Pomeau and Rica\(^17\). Using the Gross–Pitaevskii (GP) equation with a finite-range interaction (soft-core interaction), they showed that the ground state exhibits ODLRO and DLRO at a sufficiently high density of the condensate. Although this model uses a simplified interaction potential for the purposes of manageability, it is suitable for investigating supersolidity. In fact, the properties of bosons with finite-range interactions have been studied in various contexts\(^18,19,20,21,22\).

In this paper, we present a phase diagram of metastable superflow states for each phase (we call this the “stability phase diagram”) in the following) of two-dimensional soft-core bosons at zero temperature by solving the GP and the Bogoliubov equations\(^23\). Although a similar analysis has been done for a lattice system\(^24\), a continuum system has not yet been studied. We find that three phases are stable against the superflow: a superfluid phase, a supersolid phase, and a stripe phase.

Model. We use the two-dimensional GP equation with a finite range interaction\(^22,19,21,23\):

\[
\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + \int dr' V(r - r') |\Psi(r')|^2 \Psi(r) = \mu \Psi(r),
\]

where \(\Psi(r)\) is the condensate wave function, \(m\) is the atomic mass, \(V(r - r') \equiv V_0 \theta(a - |r - r'|)\) is the two-body interaction, \(V_0\) is a positive constant, \(a\) is the interaction range, and \(\theta(x)\) denotes the Heaviside step function. The chemical potential \(\mu\) is determined by the total particle number \(N\). The interaction strength of this system can be measured by a dimensionless parameter\(^22\):

\[
g \equiv m v_n a^4 V_0 / \hbar^2,
\]

where \(n_0\) is the mean-particle density. We use \(g\) as a control parameter. We assume that the solution of eq. \((1)\) is a plane wave or has a crystalline order that can be written by the Bloch wave function\(^22\):

\[
\Psi(r) = e^{\imath \mathbf{q} \cdot \mathbf{r}} \sum_{\mathcal{G}} C_{\mathcal{q} + \mathcal{G}} e^{\imath \mathcal{G} \cdot \mathbf{r}},
\]

where \(\hbar q/m\) is the velocity of the condensate, \(\mathcal{G}\) is the reciprocal lattice vector, and \(C_{\mathcal{q} + \mathcal{G}}\) is an expansion coefficient. We calculate three crystalline structures: a triangular lattice, a square lattice, and a stripe structure.
find that a square lattice structure is always dynamically responds to the case of \( q \) angular lattice, and square lattice, respectively. We have checked the convergence of the \( q \) and \( g \). In order to obtain the excitation spectrum, we solve the Bogoliubov equation:

\[
\epsilon_u(r) = Ku(r) + \int dr' V(r - r') [\Psi^*(r')\Psi(r)u(r') - \Psi(r')\Psi(r)v(r')], \tag{3}
\]
\[
\epsilon_v(r) = -Kv(r) - \int dr' V(r - r') [\Psi^*(r')\Psi^*(r)v(r') - \Psi^*(r')\Psi^*(r)u(r')], \tag{4}
\]
\[
K \equiv -\frac{\hbar^2}{2m} \nabla^2 - \mu + \int dr' V(r - r') |\Psi(r')|^2, \tag{5}
\]

where \( \epsilon \) is the excitation energy and \( u(r) \) and \( v(r) \) are excitation wave functions. Using the Bloch theorem, we can expand \( u(r) \) and \( v(r) \) in terms of the reciprocal lattice vector:

\[
u_{k,n}(r) = e^{iqr} \sum G A_{k+G,n} e^{i(k+G) \cdot r}, \tag{6}
\]
\[
v_{k,n}(r) = e^{-iqr} \sum G B_{k+G,n} e^{i(k-G) \cdot r}, \tag{7}
\]

where \( k \) is the wave number vector of the excitations, \( n \) is the band index, and \( A_{k+G,n} \) and \( B_{k+G,n} \) are expansion coefficients. Solving the GP and the Bogoliubov equations for the four assumed states, we obtain the excitation energy and local stability of each phase\(^\text{22}\). We restrict the number of expansion coefficients to 29, 73, and 81 for the stripe structure, triangular lattice, and square lattice around the origin of the reciprocal lattice space, respectively. We have checked the convergence of the present results by comparing the results with 27, 61, and 81 expansion coefficients for the stripe structure, triangular lattice, and square lattice, respectively.

**Results.** First, we show the ground state, which corresponds to the case of \( q = 0 \). In our calculation, we find that a square lattice structure is always dynamically unstable and the stripe phase is not realized at \( q = 0 \). Henceforth, we use the term “supersolid(SS) phase” only for a triangular lattice. The definitions of these phases are summarized as follows: the superfluid(SF) phase is the state in which the density of the condensate is uniform, the SS phase has a triangular lattice structure, and the stripe phase has a one-dimensional periodic structure. A typical density profile of the SS phase is shown in Fig. 1(a). Comparing the energies of the stable stationary solutions for SF and SS phases, we find that the SF (SS) phase has a lower energy than SS (SF) phase at \( g < g_c \approx 39.49 \) \((g > g_c)\). However, the chemical potentials of the SF and SS phases are not equal at \( g = g_c \). This implies that an inhomogeneous phase (= coexistence phase) is realized as the ground state in the vicinity of \( g_c \). We determine the coexistence region as 38.44 \( \leq g \leq 40.98 \); the SF phase is realized for 0 \( < g \leq 38.44 \) and the SS phase for 40.98 \( \leq g \). The result of the transition point is consistent with that of Ref. [21]22.

Next, we consider the current-flowing states with \( q \neq 0 \). The current is assumed to be parallel to the \( x \) direction \((q \equiv (q,0), q > 0)\). We do not consider coexistence phase but single phases in the following (we will discuss this point later). Figures 2 and 3 show the stability phase diagram that represents the region of single phase of metastable superflow states in the \((g, qa)\) plane.

In the SF phase, the condensate wave function and the chemical potential are given by \( \Psi(r) = \sqrt{n_0}e^{iq \cdot r} \) and \( \mu = \pi n_0 V_0 a^2 + \hbar^2 q^2 / (2m) \). Substituting these expressions into the Bogoliubov equation, we can obtain the analytical expression of the excitation spectrum in the SF phase:

\[
\epsilon_k = \frac{\hbar^2 q \cdot k}{m} + \sqrt{\frac{\hbar^2 k^2}{2m} \left[ \frac{\hbar^2 k^2}{2m} + 4\pi n_0 V_0 a^2 J_1(ka) \right]/ka}, \tag{8}
\]

where \( J_1(x) \) is a Bessel function. In the case of \( q = 0 \), this spectrum has a roton minimum when \( g \geq 15.81 \) and the roton gap vanishes at \( g \approx 46.30 \). The metastable region of the SF phase is bounded by the thin solid red
Since we cannot see the metastable region of the stripe phase in the present plot range, the magnified figure is shown in Fig. 3. The metastability of the SS phase can be judged from the excitation spectrum in the SS phase, which are obtained by numerical calculations. Figure 4(a) shows the typical excitation spectrum of the SS phase at $q = 0$. There are two gapless modes in the long wavelength limit. The lowest gapless mode is the longitudinal phonon mode and the other is the Bogoliubov mode. Since translational symmetry is broken in only one direction, the only two gapless modes exist in the long wavelength limit.

Although we have focused on the metastable states in the form of Eq. (2), there are many branches of the metastable states that cannot be written by Eq. (2) such as a coexistence phase for nonzero $q$. Further, stationary solutions including a point defect or a complex network of defects have been reported in Ref. 2. In reality, which states are realized among metastable states depends on the initial condition and experimental procedures, for example, how the velocity of a container is developed from zero as a function of time. In order to determine the final state, we need to calculate a real-time and real-space dynamics with a specified protocol. This is a future work. Our results, on the other hand, imply that we can...
reach long-lived superfluid, stripe and supersolid phases only when the values of \((g, qa)\) correspond to the regions shown in Figs. 2 and 3 for respective phases. Particularly, we see that realization of a stripe phase requires a fine tuning of the parameter \((g, qa)\) in the present model.

\[ \epsilon_0 \equiv \frac{\hbar^2}{ma^2} \] is the energy unit. The coordinates of \(\Gamma, M,\) and \(K\) points are given by \((0, 0), (2\pi/\sqrt{3}\lambda, 0),\) and \((2\pi/\sqrt{3}\lambda, 2\pi/3\lambda),\) where \(\lambda\) is a lattice constant. Similar results have been shown in Ref. [21].

**Summary and discussion.** In summary, we investigated the nature of the two-dimensional soft-core bosons at zero temperature by solving the GP and Bogoliubov equations. The superfluid, supersolid, and coexistence phases appear as the ground states. We presented the stability phase diagram, which represents the region of the homogeneous metastable states. The metastable superfluid, supersolid, and stripe phases are realized.

The problem of the presence of impurities or obstacles in the supersolid phase is a consideration for future work. The authors of Ref. [17] concluded that the superfluidity of a supersolid phase in the presence of an obstacle vanishes. However, in our calculation, a supersolid phase still exhibits a supercurrent in the presence of an obstacle. This discrepancy could be solved from the viewpoint of the stability analysis.

We thank E. Arahata, H. Watanabe, D. A. Takahashi, and G. Anagama for useful discussions. M. K. acknowledges the support of a Grant-in-Aid for JSPS Fellows (239376). This work is supported by KAKENHI (21540352) and (24543061) from JSPS and (20029007) from MEXT in Japan.

1. A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107 (1969).
2. G. V. Chester, Phys. Rev. A **2**, 256 (1970).
3. A. J. Leggett, Phys. Rev. Lett. **25**, 1543 (1970).
4. E. Kim and M. H. W. Chan, Nature (London) **427**, 225 (2004); Science **305**, 1941 (2004).
5. S. Balibar, Nature (London) **464**, 176 (2010).
6. N. Prokof’ev, Adv. Phys. **56**, 381 (2007).
7. K. Góral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002); B. Capogrosso-Sansone, C. Trefzger, M. Lewenstein, P. Zoller, and G. Pupillo, *ibid.* **104**, 125301 (2010); L. Pollet, J. D. Picon, H. P. Büchler, and M. Troyer, *ibid.* **104**, 125302 (2010).
8. N. Henkel, R. Nath, and T. Pohl, Phys. Rev. Lett. **104**, 195302 (2010); F. Cinti, P. Jain, M. Boninsegni, A. Michel, P. Zoller, and G. Pupillo, *ibid.* **105**, 135301 (2010).
9. A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, and T. Pfau, Phys. Rev. Lett. **94**, 160401 (2005).
10. M. Lu, N. Q. Burdick, S. H. Youn, and B. L. Lev, Phys. Rev. Lett. **107**, 190401 (2011).
11. K. Aikawa, A. Frisch, M. Mark, S. Baier, A. Rietzler, R. Grimm, and F. Ferlaino, Phys. Rev. Lett. **108**, 210401 (2012).
12. M. E. Fisher, M. N. Barber, and D. Jasnow, Phys. Rev. A, **8**, 1111 (1973).
13. L. D. Landau, J. Phys. (USSR) **5**, 71 (1941).
14. B. Wu and Q. Niu, Phys. Rev. A, **64**, 061603(R) (2001); New. J. Phys. **5**, 104 (2003); M. Krämer, C. Menotti, L. Pitaevskii, and S. Stringari, Eur. Phys. J. D **27**, 247 (2003).
15. R. J. Donnelly, J. A. Donnelly, and R. N. Hills, J. Low. Phys. **44**, 471 (1981).
16. J. Steinhauer, R. Ozeri, N. Katz, and N. Davidson, Phys. Rev. Lett. **88**, 120407 (2002).
where $N$ is the total particle number. We assume that the ground state wave function can be written by the Bloch wave function:

$$
\Psi(r) \equiv e^{iq \cdot r} \phi(r),
$$

where $\phi(r)$ is a periodic function that satisfies $\phi(r + n_1 a_1 + n_2 a_2) = \phi(r)$ for arbitrary integers $n_1$ and $n_2$ and primitive vectors $a_1$ and $a_2$. From this assumption, we can expand $\Psi(r)$:

$$
\Psi(r) = e^{iq \cdot r} \sum_G C_{q+G} e^{iG \cdot r},
$$

where $G$ is a reciprocal lattice vector and $C_{q+G}$ is an expansion coefficient. In the following, we abbreviate $C_{q+G}$ to $C_G$. Substituting Eq. (13) into the GP equation and multiplying both sides of the resultant equation by $\int_{u.c.} dr e^{-iG \cdot r}$,
we obtain
\[
\left[ \frac{\hbar^2}{2m}(q + G)^2 + n_0 \bar{V}(0) \right] C_G + \sum_{\Delta G \neq 0} S_{\Delta G} C_{G+\Delta G} = \mu C_G, \tag{14}
\]
\[
S_{\Delta G} \equiv \bar{V}(\Delta G) \sum_{G'} C_{G'+\Delta G} C_{G'}, \tag{15}
\]
where we introduce the Fourier transform of the two-body interaction
\[
\bar{V}(\mathbf{k}) \equiv \int d\mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} V(\mathbf{r}), \tag{16}
\]
and we used the orthonormality and the total particle number condition
\[
\frac{1}{S} \int_{u.c.} d\mathbf{r} e^{i(\mathbf{G} - \mathbf{G}')} \mathbf{r} = \delta_{\mathbf{G},\mathbf{G}'}, \tag{17}
\]
\[
n_0 \equiv \frac{N}{S} = \sum_G |C_G|^2, \tag{18}
\]
where \( S \) is the area of the unit cell and \( \int_{u.c.} d\mathbf{r} \) denotes the integral over the unit cell and \( n_0 \) is the mean-particle density. In the case of the soft-core interaction, \( \bar{V}(\mathbf{k}) \) is given by
\[
\bar{V}(\mathbf{k}) = 2\pi V_0 a^2 J_1(ka) \frac{ka}{ka}, \tag{19}
\]
where \( J_1(x) \) is a Bessel function. For example, \( S \) is given by
\[
S = \lambda^2 \quad \text{(square lattice)}, \tag{20}
\]
\[
S = \frac{\sqrt{3}}{2} \lambda^2 \quad \text{(triangular lattice)}, \tag{21}
\]
where \( \lambda \) is a lattice constant that is determined by minimizing the total energy per particle:
\[
\frac{E}{N} = \frac{\hbar^2}{2mN} \int_{u.c.} d\mathbf{r} |\nabla \Psi(\mathbf{r})|^2 + \frac{1}{2N} \int_{u.c.} d\mathbf{r} \int d\mathbf{r}' V(\mathbf{r} - \mathbf{r}')|\Psi(\mathbf{r}')|^2|\Psi(\mathbf{r})|^2
= \frac{\hbar^2}{2mn_0} \sum_G (q + G)^2 |C_G|^2 + \frac{1}{2n_0} \sum_{G_1,G_2,G_3} \bar{V}(G_1 - G_3) C_{G_1}^* C_{G_1} C_{G_2} C_{G_2} C_{G_3}. \tag{22}
\]

Here, regarding the GP equation \([14]\) as the eigenvalue equation for \( \mu \), we solve the GP equation numerically. Since the GP equation is the non-linear equation for \( C_G \), we need to solve it self-consistently. The advantage of this method is to apply the same diagonalization algorithm to solving the Bogoliubov equation described later. The detail of the procedure is as follows:

(i) Choose appropriate value of \( \lambda \).

(ii) Choose appropriate \( \{C_G\} \) as an initial condition.

(iii) Substitute \( \{C_G\} \) into \( S_{\Delta G} \) in the left-hand side of Eq. \([14]\) and diagonalize Eq. \([14]\) numerically.

(iv) Calculate the total particle energy per particle for each eigenstate.

(v) Choose \( \{C_G\} \) for the lowest energy state.

(vi) Iterate (iii)-(v) until convergence.

(vii) Choose different value of \( \lambda \) to minimize the total energy per particle.

(viii) Iterate (ii)-(vii) until convergence.
II. NUMERICAL METHOD FOR THE BOGOLIUBOV EQUATION

In this appendix, we show the numerical method for solving the Bogoliubov equation. Substituting
\[
\Psi(r, t) = e^{-i\mu t/\hbar} \left[ \Psi(r) + u(r)e^{-i\epsilon t/\hbar} - v^*(r)e^{i\epsilon t/\hbar} \right]
\] (23)
into Eq. (23) and retaining \(u(r)\) and \(v(r)\) up to \(O(u(r))\) and \(O(v(r))\), we obtain the Bogoliubov equation
\[
e\mu(r) = Ku(r) + \int dr'V(r-r') \left[ \Psi^*(r')\Psi(r)u(r') - \Psi(r')\Psi^*(r)v(r') \right],
\] (24)
\[
e\nu(r) = -Kv(r) - \int dr'V(r-r') \left[ \Psi(r')\Psi^*(r)v(r') - \Psi^*(r')\Psi^*(r)u(r') \right],
\] (25)
\[
K \equiv -\frac{\hbar^2}{2m} \nabla^2 - \mu + \int dr'V(r-r')|\Psi(r')|^2,
\] (26)
Assuming the crystalline order, we can apply the Bloch theorem to the Bogoliubov equation. \(u(r)\) and \(v(r)\) can be expanded by the reciprocal lattice vector\(^3\):
\[
u_{k,n}(r) = e^{iq_\bullet r} \sum_G A_{k,G}e^{i(k+G)\cdot r},
\] (27)
\[
v_{k,n}(r) = e^{-iq_\bullet r} \sum_G B_{k,G}e^{i(k-G)\cdot r},
\] (28)
where \(h\mathbf{k}\) is a quasi-momentum of the excitations and \(n\) is the band index. In the following, we abbreviate \(A_{k+G}\) and \(B_{k+G}\) to \(A_G\) and \(B_G\), respectively. Substituting Eqs. (27) and (28) into the Bogoliubov equation and multiplying both sides of Eqs. (24) and (25) by \(\int_{u.c.} dr e^{-iq_\bullet r}e^{-ik\cdot r}e^{-iG\cdot r}\) and \(\int_{u.c.} dr e^{iq_\bullet r}e^{-ik\cdot r}e^{iG\cdot r}\), respectively, we obtain the Bogoliubov equation for the expansion coefficients:
\[
D_G^{\pm}A_G = \sum_{G'} S_{G,G',\Delta G} A_{G'+\Delta G} - \sum_{G'} W_{G',G} B_{G'+\Delta G} = \epsilon_{k,n} A_G,
\] (29)
\[
-D_G^{\pm}B_G = \sum_{G'} S_{G,G',\Delta G} B_{G'+\Delta G} + \sum_{G'} W_{G,G'} A_{G'+\Delta G} = \epsilon_{k,n} B_G,
\] (30)
\[
D_G^{\pm}A_G \equiv \frac{\hbar^2}{2m}(q \pm k + G)^2 - \mu + n_0 \bar{V}(0) + \sum_{G'} \bar{V}(\pm k + G - G')|C_{G'}|^2,
\] (31)
\[
S_{G,G',\Delta G} = \sum_{G'} \left[ \bar{V}(\Delta G) + \bar{V}(\pm k + G - G') \right] C_{G'+\Delta G}^* C_{G'}^0,
\] (32)
\[
W_{G,G',\Delta G} = \sum_{G'} \bar{V}(\pm k + G - G')C_{2G'+\Delta G} C_{G'}^0.
\] (33)
Substituting the solution of the GP equation into Eqs. (29) and (30) and diagonalizing these equations, we obtain the excitation spectrum \(\epsilon_{k,n}\).

ACKNOWLEDGMENTS

We thank E. Arahata and D. A. Takahashi for useful comments.

---

1 kunimi@vortex.c.u-tokyo.ac.jp

2 E. Arahata and T. Nikuni, Phys. Rev. A, 79, 063606 (2009).

3 N. Sepúlveda, C. Josserand, and S. Rica, Eur. Phys. J. B 78, 439 (2010).

---

We note that the sign of \(G\) in eq. (28) will be changed by the definition of \(v\) in eq. (23).