Theory for self-bound states of dipolar Bose-Einstein condensates

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Ultracold gases of dipolar Dy have emerged as platforms where studying novel phases of matter, such as liquid droplets, poses many questions since standard theoretical methods fail to account for some of their observed properties. Here we investigate the self-bound states of dipolar Dy condensates by using general Gaussian-state ansatzes which go beyond conventional coherent-state ansatzes by including multimode squeezing. Our theory provides a transition between self-bound liquid and gas phases that agrees well with experimental observations and additionally reveals an experimentally unexplored transition in the self-bound gas region from a coherent-dominated to a squeezed-dominated phase. Our theory also allows one to extract the real part of the three-body interaction strength of the Dy atoms from the particle number distribution of the condensates. This allows us to show that the self-bound states are stabilized by the short-range three-body repulsion. Our study sheds a different light onto the properties of self-bound droplets of Bose-Einstein condensates.

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I. INTRODUCTION

Since the observation of the stable liquid droplets in dipolar condensates in the mean-field collapse regime [1,2], this novel quantum phase has received increasing attention in the community. To date, there has been rapid experimental progress in the exploration of the fundamental properties of these quantum droplets, such as their stabilization mechanism [2,3], collective excitations [2,4], self-bound states [5,6], striped states [7], and metastable states with supersolid characteristics [8–10]. Aside from dipolar systems, liquid droplets have also been observed in attractive bosonic mixtures [11–13]. In addition, droplet-droplet collisions in Bose-Bose mixtures have also been experimentally studied [14].

From the theoretical side, the stabilization mechanism of the liquid droplets is of fundamental importance. It is now widely accepted that, unlike for normal liquids, the two-body attraction is balanced at large densities by quantum fluctuations [2,3]. To the first order, quantum fluctuations can be incorporated into the Gross-Pitaevskii equation (GPE) through the Lee-Huang-Yang (LHY) correction to the condensate energy [15], leading to the so-called extended Gross-Pitaevskii equation (EGPE) [16–19]. Although the EGPE has successfully explained many experimental observations, it still shows many discrepancies as well [6]. In fact, the EGPE is affected

by an intrinsic flaw when applied to the droplet state, since the LHY correction requires the collective excitation upon the coherent ground state to be stable, which is not ensured in this case. Moreover, the coherent nature of the EGPE ground state implies that the particle number distribution (PND) is of Poissonian type, which for large particle numbers, is symmetric around the mean. This, however, is inconsistent with the asymmetric PND observed in experiments [5,6].

In this work, we revisit the stabilization-mechanism problem of the self-bound dipolar droplets by using the general Gaussian-state theory presented in Refs. [20–22], in which the many-body ground state wave functions of the condensates take the form of a multimode coherent squeezed state. As a result, quantum fluctuations are treated in a self-consistent manner within the mean-field framework. A critical ingredient in our study is the conservative three-body interaction. The inclusion of squeezing components in our theory allows us to obtain the unknown real part of the three-body coupling strength by fitting the experimentally measured PND [5]. Using this fit, we subsequently map out the phase diagram on the parameter plane formed by the relative dipolar interaction strength and the particle number. Originating from the competition between the long-range two-body attraction and the short-range three-body repulsion, we show that there exist two self-bound phases, i.e., the self-bound liquid (SBL) and the self-bound gas (SBG) phases. Remarkably, the boundary we find for the SBG-SBL transition is in good agreement with the experimental values. Although the three-body repulsion has been suggested as the mechanism that balances the two-body attraction at high densities [23–25], these GPE-based studies implicitly assume that the many-body ground state wave function of the condensate is coherent state. Consequently, the estimated real part of the three-body coupling constant is much larger than the anticipated values [3]. In contrast,

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in our work, the appearance of a squeezed component in the self-bound states gives rise to an effective enhancement of the three-body coupling constant, such that the two-body attraction is balanced at a rather smaller three-body coupling strength.

The rest of this paper is structured as follows. In Sec. II, we formulate our model and briefly introduce the Gaussian-state theory. In Sec. III, we put forward the general properties of our Gaussian ground states by factoring them into a product of single-mode displaced squeezed vacuum states. Using such factorization, we provide concise expressions for the PND and explain how to determine the three-body coupling strength of the Dy atoms. The numerical results, including the phase diagram and the condensate wave functions, are presented in Sec. IV. In Sec. V, we derive Gross-Pitaevskii-like effective equations for condensate wave functions, which show an effective enhancement of the three-body interaction, and describe well the physics in the SBG phase. Finally, we provide the conclusions in Sec. VI.

II. FORMULATION

We consider an ultracold gas of N ^{164}Dy atoms in free space. The total Hamiltonian of the system ($\hbar = 1$)

$$\hat{H} = \hat{H}_0 + \hat{H}_{2B} + \hat{H}_{3B}, \quad (1)$$

consists of single-, two-, and three-particle terms. In the second-quantized form, the single-particle Hamiltonian reads $\hat{H}_0 = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) h_0 \hat{\psi}(\mathbf{r})$, where $\hat{\psi}(\mathbf{r})$ is the field operator and $h_0 = -\nabla^2/(2M) - \mu$ with M the mass of the atoms and μ the chemical potential. The two-particle Hamiltonian takes the form

$$\hat{H}_{2B} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}). \quad (2)$$

Here, we assume that atoms interact via contact and dipolar interactions, i.e.,

$$U(\mathbf{r}) = \frac{4\pi a_s \delta(\mathbf{r})}{M} + \frac{\mu_0 \mu^2}{4\pi} \frac{1 - 3 \cos^2 \theta_{\mathbf{r}}}{r^3}, \quad (3)$$

where $a_s > 0$ is the s -wave scattering length, μ_0 is the vacuum permeability, $\mu = 9.93 \mu_B$ is the magnetic dipole moment of Dy atom with μ_B the Bohr magneton, and $\theta_{\mathbf{r}}$ is the polar angle of $\mathbf{r}$. For convenience, we introduce the relative dipolar strength $\varepsilon_{\text{dd}} = a_{\text{dd}}/a_s$ where $a_{\text{dd}} = \mu_0 \mu^2 M / 12\pi$ is the dipolar length. Finally, the three-body interaction term can be expressed as

$$\hat{H}_{3B} = \frac{g_3}{3!} \int d\mathbf{r} \hat{\psi}^{\dagger 3}(\mathbf{r}) \hat{\psi}^3(\mathbf{r}), \quad (4)$$

where g_3 is the three-body coupling constant. Although the real part of g_3 is difficult to measure experimentally, as shall be shown, it can be estimated through our theory. Without loss of generality, we assume that g_3 is real since we shall only focus on the ground state of the system.

The Gaussian-state theory assumes that the many-body wave function of the condensate takes a variational form [20–22]

$$|\Psi_{\text{GS}}\rangle = e^{\hat{\Psi}^\dagger \Sigma^z \hat{\Psi}} e^{i\hat{\Psi}^\dagger \xi \hat{\Psi}/2} |0\rangle, \quad (5)$$

where $\hat{\Psi}(\mathbf{r}) \equiv (\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}))^T$ is field operator expressed in the Nambu basis, $\Sigma^z(\mathbf{r}, \mathbf{r}') = \sigma^z \delta(\mathbf{r} - \mathbf{r}')$, σ^z being the diagonal Pauli matrix, $\Phi(\mathbf{r}) = \langle \hat{\Psi}(\mathbf{r}) \rangle = (\phi_c(\mathbf{r}), \phi_c^*(\mathbf{r}))^T$ is a variational parameter that represents the coherent part of the condensate wave function, and $\xi(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} \xi_{11}(\mathbf{r}, \mathbf{r}') & \xi_{12}(\mathbf{r}, \mathbf{r}') \\ \xi_{12}^*(\mathbf{r}', \mathbf{r}) & \xi_{11}(\mathbf{r}', \mathbf{r}) \end{pmatrix}$ is another variational parameter that characterizes the squeezing of the condensate. It should be noted that, in shorthand notation, the arguments of the exponentials in Eq. (5) should be understood to represent a matrix multiplication in Nambu space which is subsequently integrated over the position space coordinates, $\mathbf{r}$ and $\mathbf{r}'$ [26]. Hence, for example, $\hat{\Psi}^\dagger \xi \hat{\Psi} \equiv \int d\mathbf{r} d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}) \xi(\mathbf{r}, \mathbf{r}') \hat{\Psi}(\mathbf{r}')$, but only on that equation.

Since different ξ 's may lead to the same Gaussian state, the variational parameter ξ contains redundancies [20,21]. In order to remove these, we introduce the covariance matrix $\Gamma(\mathbf{r}, \mathbf{r}') = \langle \{\delta\hat{\Psi}(\mathbf{r}), \delta\hat{\Psi}^\dagger(\mathbf{r}')\} \rangle$ defined in both the Nambu and the coordinate spaces, where $\delta\hat{\Psi} = \hat{\Psi} - \Phi$ is the fluctuation field. We note that Γ and ξ are connected through the relation [20]

$$\Gamma = S S^\dagger, \quad (6)$$

where $S \equiv e^{i\Sigma^z \xi}$ represents a transformation satisfying $S \Sigma^z S^\dagger = \Sigma^z$. Moreover, the diagonal and the off-diagonal blocks of Γ can be further expressed as

$$\Gamma_{11}(\mathbf{r}, \mathbf{r}') = \Gamma_{22}(\mathbf{r}', \mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}') + 2G(\mathbf{r}, \mathbf{r}'), \quad (7a)$$

$$\Gamma_{12}(\mathbf{r}, \mathbf{r}') = \Gamma_{21}^*(\mathbf{r}', \mathbf{r}) = 2F(\mathbf{r}, \mathbf{r}'), \quad (7b)$$

where

$$G(\mathbf{r}, \mathbf{r}') = \langle \delta\hat{\psi}^\dagger(\mathbf{r}') \delta\hat{\psi}(\mathbf{r}) \rangle, \quad (8a)$$

$$F(\mathbf{r}, \mathbf{r}') = \langle \delta\hat{\psi}(\mathbf{r}) \delta\hat{\psi}^\dagger(\mathbf{r}') \rangle, \quad (8b)$$

are the normal and the anomalous correlation functions, respectively.

To proceed further, we make use of the Wick theorem on $\hat{H}$, which, to quadratic order in $\delta\hat{\Psi}$, gives rise to the mean-field Hamiltonian [26] (we omit spatial integration)

$$\hat{H}_{\text{MF}} = E_0 + (\delta\hat{\Psi}^\dagger \eta[\phi, \Gamma] + \text{H.c.}) + \frac{1}{2} : \delta\hat{\Psi}^\dagger \mathcal{H}[\phi, \Gamma] \delta\hat{\Psi} :. \quad (9)$$

Here, $:\hat{\mathcal{O}}:$ denotes normal ordering of the operator $\hat{\mathcal{O}}$ with respect to the Gaussian state (5), and the derivations of the ground-state energy E_0 , the linear term $\eta[\phi, \Gamma]$ and the quadratic term $\mathcal{H}[\phi, \Gamma] \equiv \begin{pmatrix} \mathcal{E}[\phi, \Gamma] & \Delta[\phi, \Gamma] \\ \Delta^\dagger[\phi, \Gamma] & \mathcal{E}^*[\phi, \Gamma] \end{pmatrix}$ are provided in Appendix [26]. The ground-state solutions, $\{\phi, \Gamma\}$, can be obtained by evolving the imaginary-time equations of motion [20,22]

$$\partial_\tau \Phi = -\Gamma \begin{pmatrix} \eta \\ \eta^* \end{pmatrix}, \quad (10a)$$

$$\partial_\tau \Gamma = \Sigma^z \mathcal{H} \Sigma^z - \Gamma \mathcal{H} \Gamma, \quad (10b)$$

which converge for a sufficiently large imaginary time τ . The numerical procedures for evolving Eq. (10) are detailed in Appendix [26].

III. GENERAL PROPERTIES OF THE GROUND STATES

From a physical point of view, it is very instructive to show that our general Gaussian state (5) can always be written as a product of single-mode displaced squeezed vacuum states. To this end, let us first eliminate the redundancy in ξ with an approach based on group theory [21]. The transformations S and S' give rise to the same Gaussian state if

$$SS^\dagger = S'S'^\dagger. \quad (11)$$

Consider now an S' related to S by an infinitesimal transformation, that is, $S' = e^{i\Sigma^z \delta\xi} e^{i\Sigma^z \delta\xi} \approx e^{i\Sigma^z \delta\xi} (1 + i\Sigma^z \delta\xi)$, where $\delta\xi$ is an infinitesimal generator. The condition (11) becomes $[\delta\xi, \Sigma^z] = 0$, which implies that a transformation generated by any diagonal generator does not change the covariance matrix, thus leading to the same Gaussian state. As a result, we can remove the redundancy by fixing the diagonal elements of $\xi(\mathbf{r}, \mathbf{r}')$, which we set to zero, obtaining an off-diagonal generator

$$\xi(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} 0 & \xi_{12}(\mathbf{r}, \mathbf{r}') \\ \xi_{12}^*(\mathbf{r}', \mathbf{r}) & 0 \end{pmatrix}, \quad (12)$$

which generates a redundancy-free variational state (5). Then, noting that the complex function $\xi_{12}(\mathbf{r}, \mathbf{r}')$ is symmetric under the exchange of its arguments, we can use Takagi diagonalization [27] in the space of square-integrable functions to write it as

$$\xi_{12}(\mathbf{r}, \mathbf{r}') = -i \sum_{j=1}^{\infty} \bar{\phi}_{s,j}(\mathbf{r}) d_j \bar{\phi}_{s,j}(\mathbf{r}'), \quad (13)$$

where all eigenvalues d_j are positive and all eigenvectors $\bar{\phi}_{s,j}(\mathbf{r})$ satisfy the orthonormal conditions $\int d\mathbf{r} \bar{\phi}_{s,i}^* \bar{\phi}_{s,j} = \delta_{ij}$. Without loss of generality, we assume that the d_j 's are sorted in descending order with respect to the index j . The Gaussian state (5) can then be factorized into the form

$$|\Psi_{\text{GS}}\rangle = e^{\sqrt{N_c}(\hat{b}_c^\dagger - \hat{b}_c)} \prod_{j=1}^{\infty} e^{\frac{1}{2} d_j (\hat{b}_{s,j}^{\dagger 2} - \hat{b}_{s,j}^2)} |0\rangle, \quad (14)$$

where $\hat{b}_{s,j} = \int d\mathbf{r} \hat{\psi}(\mathbf{r}) \bar{\phi}_{s,j}^*(\mathbf{r})$ is the annihilation operator for the j th squeezed mode, d_j clearly has the meaning of a squeezing factor, such that $N_{s,j} = \sinh^2 d_j$ is the corresponding contribution to the mean occupation number coming from such mode. On the other hand, $N_c = \int d\mathbf{r} |\phi_c(\mathbf{r})|^2$ is the contribution of the coherent part of the condensate to the mean particle number, and $\hat{b}_c = \int d\mathbf{r} \hat{\psi}(\mathbf{r}) \bar{\phi}_c^*(\mathbf{r})$ is the annihilation operator associated to the normalized coherent mode function $\bar{\phi}_c(\mathbf{r}) = \phi_c(\mathbf{r})/\sqrt{N_c}$. Note that the $\hat{b}_{s,j}$'s form a complete set of annihilation operators, and hence $\hat{b}_c$ is not independent of them, as we highlight shortly.

Through the covariance matrix Γ , the normal and the anomalous correlation functions take the diagonal form

$$G(\mathbf{r}, \mathbf{r}') = \sum_{j=1}^{\infty} N_{s,j} \bar{\phi}_{s,j}(\mathbf{r}) \bar{\phi}_{s,j}^*(\mathbf{r}'), \quad (15a)$$

$$F(\mathbf{r}, \mathbf{r}') = \sum_{j=1}^{\infty} \sqrt{N_{s,j}(N_{s,j} + 1)} \bar{\phi}_{s,j}(\mathbf{r}) \bar{\phi}_{s,j}(\mathbf{r}'). \quad (15b)$$

Equations (7), (14), and (15) establish the explicit relation between the covariance matrix and the squeezed component of the variational state: once a converged ground-state solution $\{\phi, \Gamma\}$ is obtained numerically, we diagonalize $G(\mathbf{r}, \mathbf{r}')$ or $F(\mathbf{r}, \mathbf{r}')$ to find the squeezed modes $\bar{\phi}_{s,j}(\mathbf{r})$ and the occupation numbers $N_{s,j}$.

A. Particle number distribution

Interestingly, in the presence of the squeezed component, the PND and equivalently the quantum statistics of $|\Psi_{\text{GS}}\rangle$ may differ from that of a coherent state significantly. To see this, we expand the coherent mode $\hat{b}_c$ using the squeezed modes as

$$\hat{b}_c^\dagger = \sum_{j=1}^S \alpha_j \hat{b}_{s,j}^\dagger + \alpha_\perp \hat{b}_\perp^\dagger, \quad (16)$$

where $\alpha_j = \int d\mathbf{r} \bar{\phi}_{s,j}^*(\mathbf{r}) \bar{\phi}_c(\mathbf{r})$, $\alpha_\perp^2 = 1 - \sum_j |\alpha_j|^2$, and $\hat{b}_\perp$ represents the mode that is perpendicular to all $\hat{b}_{s,j}$. For practical purposes, we have introduced a truncation S on the total number of squeezed modes since it is found that $N_{s,j}$ decays rapidly as j increases. The variational ground state (14) can now be expressed as

$$|\Psi_{\text{GS}}\rangle = e^{\sqrt{N_c} \alpha_\perp (\hat{b}_\perp^\dagger - \hat{b}_\perp)} \prod_{j=1}^S e^{\sqrt{N_c} (\alpha_j \hat{b}_{s,j}^\dagger - \alpha_j^* \hat{b}_{s,j})} e^{\frac{1}{2} d_j (\hat{b}_{s,j}^{\dagger 2} - \hat{b}_{s,j}^2)} |0\rangle. \quad (17)$$

The PND of the coherent mode $\hat{b}_\perp$ is of the Poissonian type

$$p_\perp(\ell) = e^{-N_c |\alpha_\perp|^2} \frac{(N_c |\alpha_\perp|^2)^\ell}{\ell!}, \quad (18)$$

where ℓ is the occupation number in bosonic mode. For the coherent-squeezed mode $\hat{b}_{s,j}$, the PND is [28]

$$p_{s,j}(\ell) = \frac{(\frac{1}{2} \tanh d_j)^\ell}{\ell! \cosh d_j} [H_\ell[\gamma_j (\sinh 2d_j)^{-1/2}]]^2 \times \exp \left[-|\alpha_j|^2 - \frac{1}{2} (\alpha_j^{*2} + \alpha_j^2) \tanh d_j \right], \quad (19)$$

where $\gamma_j = \alpha_j \cosh d_j + \alpha_j^* \sinh d_j$ and $H_\ell(x)$ are Hermite polynomials. Now, the PND of $|\Psi_{\text{GS}}\rangle$ can then be found recursively as follows. Let $P_j(n)$ denote the PND of the state containing the first j squeezed modes, the PND containing first $j+1$ squeezed modes can then be expressed as

$$P_{j+1}(n) = \sum_{\ell=0}^n P_j(n-\ell) p_{s,j+1}(\ell), \quad (20)$$

where $P_0(n) \equiv p_\perp(n)$. Applying the relation (20) successively leads to the total PND, which we denote by $P_S(n)$.

In general, $P_S(n)$ is peaked at roughly $n \approx N_c$. To the left of this peak, the PND is mainly determined by the Poisson distribution (18) of the coherent part of the condensate, such that $P_S(n)$ increases abruptly as n approaches N_c . In contrast, to the right of the peak, $P_S(n)$ shows a long tail reaching large n due to the squeezing component of the condensate [28]. As a result, $P_S(n)$ becomes asymmetric around N_c , which is in striking contrast to the PND of a coherent state.

FIG. 1. Red triangles shows the PND for the state obtained with the parameters $N^* = 790$, $g_3^* = 6.73 \times 10^{-40} \hbar \text{ m}^6/\text{s}$, and $\varepsilon_{dd} = 2.04$ (corresponding to a magnetic field $B = 6.624 \text{ G}$). The histogram represent the experimental data [5].

B. Determination of g_3

In Ref. [5], the PNDs of the condensates were experimentally measured under various magnetic fields or, equivalently, ε_{dd} 's. Because the measured PNDs were asymmetric around the mean particle number, they were fitted with a function that is the convolution of a Gaussian and a Maxwell-Boltzmann distribution in Ref. [5]. Here we attribute the measured PNDs to that of the Gaussian state $|\Psi_{GS}\rangle$ and fit the measured PNDs with $P_S(n)$. Specifically, for every PND obtained under a given magnetic field in Ref. [5], we have carried out extensive fittings by systematically varying the values of N and g_3 . It is found that the experimentally measured PNDs are broader than that obtained with $P_S(n)$, which might originate from the detection noise and the thermal fluctuations of the condensates in the evaporation. The best fit, as shown in Fig. 1, is achieved under the magnetic field $B = 6.624 \text{ G}$ with fitting parameters $N^* = 790$ and $g_3^* = 6.73 \times 10^{-40} \hbar \text{ m}^6/\text{s}$, where N^* roughly agrees with the experimentally measured mean number of atoms. Interestingly, this value of g_3^* is about one order of magnitude smaller than that used in previous works [23], and is therefore more favorable [3]. Unless otherwise stated, the value of the three-body coupling strength will always be fixed to g_3^* below.

IV. PHASE DIAGRAM

In Fig. 2(a), we map out the coherent-component fraction $f_c \equiv N_c/N$ of the condensate in the (ε_{dd}, N) parameter plane. In order to reveal more details, we show the typical ε_{dd} and N dependence of f_c in Fig. 2(b) and the ε_{dd} dependence of the kinetic energy E_{kin} , the two-body interaction energy E_{2B} , and the three-body interaction energy E_{3B} in Fig. 2(c). The detailed expressions for these energy components can be found in Appendix [26]. We note that for the parameters covered by our numerical calculations, we always have $E_{2B} < 0$. Moreover, since the peak density n_{peak} and the radial $1/e^2$ width σ_ρ (or the axial $1/e^2$ width σ_z) are of interest to

FIG. 2. (a) Distribution of the coherent-component fraction on the (ε_{dd}, N) parameter plane. The black dashed line marks the boundary across which the value of f_c changes abruptly. The white dash-dotted line denote boundary between the self-bound state and the expanding state. Empty triangles represent the experimental data for the critical particle number. (b) The solid line shows the ε_{dd} dependence of f_c for $N = 1000$ and dashed line plots the N dependence of f_c for $\varepsilon_{dd} = 1.92$. (c) The ε_{dd} dependence of E_{kin} , $|E_{2B}|$, and E_{3B} for $N = 1000$.

experimentalists, we also map out the values of $\log n_{\text{peak}}$ and σ_ρ on the (ε_{dd}, N) parameter plane in Fig. 3. An immediate observation is that all three figures share the same structure. Namely, the parameter plane is divided into three parts, representing the expanding-gas (EG) region, the SBG phase, and the SBL phase, respectively. For parameters in the EG region, condensates cannot exist in the form of a self-bound state in free space. Therefore, it is not of interest to the present work.

In the SBG phase, the attractive interaction or the atom number is large enough for the condensate to form a self-bound state. Because the density is still relatively low [see Fig. 3(a)], the condensate remains in the gas phase. An important feature of the SBG phase is that the squeezed component is always dominated by a single squeezed mode (see Fig. 5). More interestingly, the SBG phase can be further divided into two subregions by the dotted line in Fig. 2(a): (i) To the left of this boundary, the coherent-component fraction vanishes completely, such that the condensate is in a single-mode squeezed vacuum state, similarly to that of a trapped weakly attractive condensate [22]. (ii) To the right of the dotted line, the ground state of the condensate is a squeezed coherent state in which f_c can be as high as around 0.64. Analyzing the ε_{dd} dependence of the ground-state energy $E_0 (= E_{\text{kin}} + E_{2B} + E_{3B})$ further reveals that the transition between the squeezed vacuum and the squeezed coherent states is of third order, since the third derivative of E_0 with respect to ε_{dd} is discontinuous. This transition reflects the fact that the appearance of the coherent component breaks the Z_2 symmetry possessed by the pure

FIG. 3. Distribution of the peak density $\log n_{\text{peak}}$ and the radial width σ_ρ of the condensate on the (ϵ_{dd}, N) plane. Here n_{peak} and σ_ρ are in units of m^{-3} and μm , respectively. The dashed and dotted lines mark the corresponding phase boundaries in Fig. 2(a).

squeezed states. Physically, increasing ϵ_{dd} or N enhances both two-body and three-body interactions, which shrinks the condensate and leads to a higher density (see Fig. 3). It turns out that a coherent condensate is more energetically favorable in the high density regime, where the squeezed atoms are turned into coherent ones. This mechanism can be further confirmed by deliberately lowering the value of g_3 in numerical calculations. It is found that for the same set of ϵ_{dd} and N , the coherent-component fraction monotonically increases when g_3 is lowered.

As one further increases ϵ_{dd} or N , the three-body repulsion becomes more relevant, such that f_c increases abruptly and the coherent part of the condensate becomes dominant ($f_c \gtrsim 0.8$). The system then enters the SBL phase through a first-order phase transition. Across the phase boundary, as shown in Fig. 3, n_{peak} and σ_ρ also experience an abrupt change. We point out that the values of n_{peak} and σ_ρ in the SBL phase are also in rough agreement with experiments [5]. Moreover, to further test our theory, we numerically compute the critical atom number for the recent ^{162}Dy experiment [6]. As shown in Fig. 4, our results demonstrate better agreement with experimental data than those obtained with the EGPE.

To gain more insight into the gas-liquid transition, we examine the number of the squeezed modes by introducing the so-called notably-populated squeezed modes (NPSMs). Specifically, the j th squeezed mode is an NPSM if $N_{s,j}/\sum_i N_{s,i} \geq 0.5\%$. In Fig. 5, we present the distribution of the number of the NPSMs in the $\epsilon_{dd}N$ plane, where the SBL-SBG boundary is sharply defined. The SBG phase is dominated by a single squeezed mode; while across the gas-liquid boundary, the coherent component becomes dominant and the number of NPSMs increases abruptly. Physically, the

FIG. 4. Critical atom number for the SBL phase of the ^{162}Dy condensates. Solid line is computed with the GST, in which we have used the same three-body coupling constant as that of ^{164}Dy atoms. Filled triangles and dashed line (both are taken from Ref. [6]) represent the experimental data and the EGPE result, respectively. The a_{dd} value used in the EGPE simulations is slightly different from the actual one, however, the critical atom number caused by this discrepancy is negligible [6].

squeezing in the SBG phase originates from the overall attractive two-body interactions, same as that in the condensate with pure s -wave interaction [22]. On the other hand, the squeezing in the SBL phase represents the depletion of the condensate that is induced by the three-body repulsion. Indeed, it is verified that the fraction of the squeezed component increases if we increase g_3 or, equivalently, decrease ϵ_{dd} .

We now examine the density profiles which consist of the coherent part $n_c(\mathbf{r}) = |\phi_c(\mathbf{r})|^2$ and the squeezed part $n_s(\mathbf{r}) = G(\mathbf{r}, \mathbf{r})$. Due to axial symmetry of the condensate, both n_c and n_s are cylindrically symmetric. In Fig. 6, we plot the density profiles along the radial $\rho = \sqrt{x^2 + y^2}$ and the z directions for both coherent and squeezed components with $N = 700$ and for various ϵ_{dd} 's. In addition, because the density is symmetric about the $z = 0$ plane, only the density profiles for $z \geq 0$ are plotted.

For the coherent component, n_c always reaches its peak value at the center of the condensate. It then monotonically

FIG. 5. Contour plot for the number of the NPSMs.

FIG. 6. Density profiles $n_c(\rho, 0)$ (a), $n_c(0, z)$ (b), $n_s(\rho, 0)$ (c), $n_s(0, z)$ (d), $n_t(\rho, 0)$ (e), $n_t(0, z)$ (f) for $N = 700$ and $\varepsilon_{dd} = 2.08$ (solid lines), 1.92 (dashed lines), 1.67 (dash-dotted lines), and 1.33 (dotted lines).

decreases along both the radial and the axial directions. In addition, as ε_{dd} increases, the peak value of n_c also grows along with the increase of f_c . As to the squeezed component, similar to the behavior of n_c , n_s also reaches its peak at the condensate center when ε_{dd} is small. However, for large ε_{dd} , the value of n_s at the condensate center drops such that both $n_s(\rho, 0)$ and $n_s(0, z)$ are not monotonic. Physically, this can be understood by noting the total density, $n_t = n_c + n_s$, is always maximized at the center of the condensate [Figs. 6(e) and 6(f)]. As a result, the three-body repulsion is strongest at the center of the condensate which locally turns the squeezed component into the coherent one. Now, the structure of a liquid droplet can be roughly described as follows: the high-density coherent component forms the liquid core of the condensate; while the low-density squeezed component constitutes a gas shell surrounding the liquid core.

V. EFFECTIVE EQUATIONS FOR THE SELF-BOUND STATES

In principle, we may derive effective equations for the ground-state spatial modes ϕ_c and $\{\phi_{s,j}\}_{j=1}^S$ by minimizing the ground-state energy E_0 under the constraints that the unnormalized squeezed modes $\phi_{s,j} = \sqrt{N_{s,j}}\tilde{\phi}_{s,j}$ are mutually orthogonal. This however becomes very cumbersome deep inside the SBL phase, since the number of the squeezed modes

could be very large. We notice that deep into the SBL phase, most atoms are in a coherent state, while in the SBG phase the squeezed component is dominated by a single mode, i.e., $S = 1$. As a result, deep into the SBL phase, the ground state is described by a single macroscopic wave function $\phi_c(\mathbf{r})$ that obeys the conventional GPE. In the SBG phase, both coherent and squeezed condensates contain a macroscopic number of particles, which are characterized by two macroscopic wave functions $\chi(\mathbf{r}) \equiv (\phi_c(\mathbf{r}), \phi_s(\mathbf{r}))^T$, where $\phi_s(\mathbf{r}) \equiv \phi_{s,1}(\mathbf{r})$ describes the mode with the largest squeezing. The conditions $\delta E_0 / \delta \chi^\dagger = 0$ then give rise to the coherent-squeezed-state GPEs [26]

$$\left[h_0 I + \mathcal{M}^{(2)}(\mathbf{r}) + \frac{g^3}{2} \mathcal{M}^{(3)}(\mathbf{r}) \right] \chi(\mathbf{r}) = 0, \quad (21)$$

where I is a 2×2 identity matrix, while

$$\mathcal{M}^{(2)}(\mathbf{r}) = \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \begin{pmatrix} n_1(\mathbf{r}') & n_{sc}(\mathbf{r}') \\ n_{sc}(\mathbf{r}') & n_3(\mathbf{r}') \end{pmatrix}, \quad (22a)$$

$$\mathcal{M}^{(3)}(\mathbf{r}) = \begin{pmatrix} n_3^2 + \phi_s^{*2} \phi_c^2 & 3n_2 \phi_s \phi_c^* \\ 2n_{9/2} \phi_c \phi_s^* & 3n_1 n_5 + 3\phi_c^{*2} \phi_s^2 \end{pmatrix}, \quad (22b)$$

are the mean fields induced by the two- and three-body interactions, respectively. Here, we have introduced the notation $n_q = |\phi_c|^2 + q|\phi_s|^2$ and $n_{sc} = 2\text{Re}(\phi_s^* \phi_c)$. We point out that the diagonal elements of $\mathcal{M}^{(2)}$ receive a contribution from intra-state interactions and from inter-state Hartree interactions; in contrast, the off-diagonal terms originate from inter-state Fock and pairing interactions [26].

To appreciate the physical significance of Eqs. (21), let us consider the simplest cases by assuming that the condensate is either in a pure coherent state or in a single-mode squeezed vacuum state. For either case, Eqs. (21) reduce to a unified form:

$$\left[h_0 + c_2 \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') |\varphi(\mathbf{r}')|^2 + c_3 \frac{g^3}{2} |\varphi(\mathbf{r})|^4 \right] \varphi(\mathbf{r}) = 0,$$

where $c_2 = c_3 = 1$ if $\varphi \equiv \phi_c$ and $c_2 = 3$ and $c_3 = 15$ if $\varphi \equiv \phi_s$. Remarkably, although both two- and three-body interaction strengths of the squeezed state are enhanced compared to those of the coherent state ansatz, the enhancement of the three-body interaction strength is comparatively larger. As shown in the expression of E_{3B} in Appendix [26], this large enhancement to the three-body interaction strength originates from the fact that the combination of squeezing and three-body interaction yields more terms when applying the Wick theorem.

We have performed extensive numerical calculations to check the validity of these effective equations in the SBG phase. It is found that away from the gas-liquid boundary the results obtained with the effective equations are in perfect agreement with those computed using Eqs. (10). In contrast, close to the gas-liquid boundary, because the number of squeezed modes increases rapidly, the effective equations become less accurate (see Appendix [26] for details).

VI. DISCUSSION AND CONCLUSION

As analyzed in our previous work [22], if we sequentially solve Eqs. (10a) and (10b) iteratively starting with a pure coherent state, the EGPE is merely the resulting equation

after the first iteration. Therefore the EGPE is applicable only when the condensate is dominated by the coherent component, which excludes its application to the SBG phase. Even for the coherent-component-dominant SBL phase one should be very careful about the validity of the EGPE. In fact, in its current form, the EGPE only takes into account the quantum fluctuations induced by two-body interactions, while quantum fluctuations in the SBL phase are induced by three-body repulsion. To further confirm this, we have performed numerical simulations with $g_3 = 0$. We have found that condensates always collapse for all parameters covered by Fig. 2(a). This result clearly suggests that the quantum fluctuations associated with two-body interactions are insufficient to balance two-body attraction.

We note that three-body repulsion was previously considered as the source that stabilizes the two-body attraction in Refs. [23–25]. However, to match the experimental measurements, the estimated three-body coupling constant using the GPE is much higher than the expected value [5]. Within the Gaussian-state theory, the appearance of the squeezed component leads to the unusual enhancement to the three-body coupling constant such that the two-body attraction is balanced at a rather smaller g_3 . For parameters deep inside the SBL phase where the squeezing becomes negligibly small, it has been verified that the GPE with three-body repulsion can lead to the same results as those obtained with Eqs. (10) [26].

In summary, we have studied the self-bound states of dipolar condensates by using a general Gaussian-state theory that allows us to treat quantum fluctuations in a self-consistent manner. Aside from the SBL droplet phase, we have been able to predict the existence of a SBG phase. We have also shown that the gas-liquid transition is induced by the competition between long-range two-body attraction and short-range

three-body repulsion. Unlike the conventional theory based on coherent states, a relevant squeezed component emerges in the ground states of both phases, ought to distinct physical origins: it is induced by the two-body attraction (three-body repulsion) in the SBG (SBL) phase. The appearance of the squeezed component in the self-bound states is crucial as (particularly in the SBL phase) it allows the three-body repulsion to balance the two-body attraction even with a relatively small three-body coupling constant.

As for the possibility of testing our results experimentally, we note that the squeezed-component-dominant SBG phase can be detected by measuring the second-order correlation function of the gas, as it exhibits distinct quantum statistics from that of the coherent-component-dominant SBL phase [22]. In addition, carefully examining the PND of the condensates would also reveal the squeezed nature of the SBG phase. In the future, we shall further study the dynamical formation of the self-bound states. We believe our study opens up a broad avenue to explore brand new macroscopic quantum states in cold atom systems.

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APPENDIX A: MEAN-FIELD HAMILTONIANS

Here we outline the derivation of the mean-field Hamiltonian (5). To this end, we substitute the expansion $\psi(\mathbf{r}) = \phi(\mathbf{r}) + \delta\psi(\mathbf{r})$ into the total Hamiltonian H , which leads to

$$H_0 = \int d\mathbf{r} \{ \phi^*(\mathbf{r}) h_0 \phi(\mathbf{r}) + [\delta\psi^\dagger(\mathbf{r}) h_0 \phi(\mathbf{r}) + \text{H.c.}] + \delta\psi^\dagger(\mathbf{r}) h_0 \delta\psi(\mathbf{r}) \}, \quad (\text{A1})$$

$$\begin{aligned} H_{2B} = \int d\mathbf{r} d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') & \left\{ \frac{1}{2} |\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2 + [|\phi(\mathbf{r}')|^2 \phi(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}) + \text{H.c.}] \right. \\ & + |\phi(\mathbf{r}')|^2 \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) + \phi^*(\mathbf{r}') \phi(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}') + \frac{1}{2} [\phi(\mathbf{r}') \phi(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}') + \text{H.c.}] \\ & \left. + [\phi(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') + \text{H.c.}] + \frac{1}{2} \delta\psi^\dagger(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') \delta\psi(\mathbf{r}) \right\}, \quad (\text{A2}) \end{aligned}$$

$$\begin{aligned} H_{3B} = g_3 \int d\mathbf{r} & \left\{ \frac{1}{3!} |\phi(\mathbf{r})|^6 + \frac{1}{2} [|\phi(\mathbf{r})|^4 \phi(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}) + \text{H.c.}] \right. \\ & + \frac{3}{2} |\phi(\mathbf{r})|^4 \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) + \frac{1}{2} [|\phi(\mathbf{r})|^2 \phi^2(\mathbf{r}) \delta\psi^{\dagger 2}(\mathbf{r}) + \text{H.c.}] \\ & + \frac{1}{3!} [\phi^3(\mathbf{r}) \delta\psi^{\dagger 3}(\mathbf{r}) + 9|\phi(\mathbf{r})|^2 \phi(\mathbf{r}) \delta\psi^{\dagger 2}(\mathbf{r}) \delta\psi(\mathbf{r}) + \text{H.c.}] \\ & + \frac{1}{2} [\phi^2(\mathbf{r}) \delta\psi^{\dagger 3}(\mathbf{r}) \delta\psi(\mathbf{r}) + 3|\phi(\mathbf{r})|^2 \delta\psi^{\dagger 2}(\mathbf{r}) \delta\psi^2(\mathbf{r}) + \phi^{*2}(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}) \delta\psi^3(\mathbf{r})] \\ & \left. + \frac{1}{2} [\phi(\mathbf{r}) \delta\psi^{\dagger 3}(\mathbf{r}) \delta\psi^2(\mathbf{r}) + \text{H.c.}] + \frac{1}{3!} \delta\psi^{\dagger 3}(\mathbf{r}) \delta\psi^3(\mathbf{r}) \right\}. \quad (\text{A3}) \end{aligned}$$

After applying the Wick's theorem with respect to the Gaussian state $|\Psi_{\text{GS}}\rangle$, we obtain the mean-field Hamiltonian

$$H_{\text{MF}} = E_0 + (\delta\psi^\dagger \eta + \text{H.c.}) + t \frac{1}{2} : \delta\psi^\dagger \mathcal{H} \delta\psi :, \quad (\text{A4})$$

where $E_0 = E_{\text{kin}} + E_{2B} + E_{3B}$ is the average energy of the system with

$$\begin{aligned} E_{\text{kin}} &= \int d\mathbf{r} [\phi^*(\mathbf{r}) h_0 \phi(\mathbf{r}) + \langle \delta\psi^\dagger(\mathbf{r}) h_0 \delta\psi(\mathbf{r}) \rangle], \\ E_{2B} &= \int d\mathbf{r} d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \left\{ \frac{1}{2} |\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2 + \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}') \rangle \left[|\phi(\mathbf{r}')|^2 + \frac{1}{2} \langle \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle \right] \right. \\ &\quad + \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}') \rangle \left[\phi^*(\mathbf{r}') \phi(\mathbf{r}) + \frac{1}{2} \langle \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle \right] \\ &\quad \left. + \text{Re} \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi^\dagger(\mathbf{r}') \rangle \left[\phi(\mathbf{r}') \phi(\mathbf{r}) + \frac{1}{2} \langle \delta\psi(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle \right] \right\}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} E_{3B} &= g_3 \int d\mathbf{r} \left[\frac{1}{3!} |\phi(\mathbf{r})|^6 + \frac{3}{2} |\phi(\mathbf{r})|^4 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle + \text{Re} |\phi(\mathbf{r})|^2 \phi^2(\mathbf{r}) \langle \delta\psi^{\dagger 2}(\mathbf{r}) \rangle \right. \\ &\quad + 3 \text{Re} \phi^2(\mathbf{r}) \langle \delta\psi^{\dagger 2}(\mathbf{r}) \rangle \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle + 3 |\phi(\mathbf{r})|^2 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle^2 + \frac{3}{2} |\langle \delta\psi^2(\mathbf{r}) \rangle|^2 |\phi(\mathbf{r})|^2 \\ &\quad \left. + \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle^3 + \frac{3}{2} |\langle \delta\psi^2(\mathbf{r}) \rangle|^2 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle \right] \end{aligned} \quad (\text{A6})$$

being the kinetic, the two-body interaction, and the three-body interaction energies, respectively. The linear driving term is

$$\begin{aligned} \eta(\mathbf{r}) &= h_0 \phi(\mathbf{r}) + \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \{ [|\phi(\mathbf{r}')|^2 + \langle \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle] \phi(\mathbf{r}) + \langle \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle \phi(\mathbf{r}') + \langle \delta\psi(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle \phi^*(\mathbf{r}') \} \\ &\quad + g_3 \left\{ \frac{1}{2} \left[|\phi(\mathbf{r})|^4 + \frac{1}{2} \langle \delta\psi^{\dagger 2}(\mathbf{r}) \rangle \phi^2(\mathbf{r}) + \frac{3}{2} |\langle \delta\psi^2(\mathbf{r}) \rangle|^2 + 3 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle (|\phi(\mathbf{r})|^2 + \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle) \right] \phi(\mathbf{r}) \right. \\ &\quad \left. + 3 \left[\frac{1}{2} |\phi(\mathbf{r})|^2 + \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle \right] \langle \delta\psi^2(\mathbf{r}) \rangle \phi^*(\mathbf{r}) \right\}. \end{aligned} \quad (\text{A7})$$

The mean-field Hamiltonian $\mathcal{H} = \begin{pmatrix} \mathcal{E} & \Delta \\ \Delta^\dagger & \mathcal{E}^* \end{pmatrix}$ is determined by

$$\begin{aligned} \mathcal{E} &= h_0 + \delta(\mathbf{r} - \mathbf{r}') \int d\mathbf{r}_1 U(\mathbf{r} - \mathbf{r}_1) [|\phi(\mathbf{r}_1)|^2 + \langle \delta\psi^\dagger(\mathbf{r}_1) \delta\psi(\mathbf{r}_1) \rangle] + U(\mathbf{r} - \mathbf{r}') [\phi^*(\mathbf{r}') \phi(\mathbf{r}) + \langle \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}') \rangle] \\ &\quad + \frac{3}{2} g_3 \delta(\mathbf{r} - \mathbf{r}') [|\phi(\mathbf{r})|^4 + 4 |\phi(\mathbf{r})|^2 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle + 2 \text{Re} \langle \delta\psi^{\dagger 2}(\mathbf{r}) \rangle \phi^2(\mathbf{r}) + 2 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle^2 + |\langle \delta\psi^2(\mathbf{r}) \rangle|^2] \end{aligned} \quad (\text{A8})$$

and

$$\begin{aligned} \Delta &= U(\mathbf{r} - \mathbf{r}') [\phi(\mathbf{r}') \phi(\mathbf{r}) + \langle \delta\psi(\mathbf{r}') \delta\psi(\mathbf{r}) \rangle] + g_3 \delta(\mathbf{r} - \mathbf{r}') [|\phi(\mathbf{r})|^2 \phi^2(\mathbf{r}) + 3 \phi^2(\mathbf{r}) \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle \\ &\quad + 3 |\phi(\mathbf{r})|^2 \langle \delta\psi^2(\mathbf{r}) \rangle + 3 \langle \delta\psi^\dagger(\mathbf{r}) \delta\psi(\mathbf{r}) \rangle \langle \delta\psi^2(\mathbf{r}) \rangle]. \end{aligned} \quad (\text{A9})$$

APPENDIX B: SOLVING EOM BY HANKEL TRANSFORMATIONS

In this section, we solve EOM (6) projected in the angular momentum basis by Hankel transformations. In the basis $e^{im\varphi}/\sqrt{2\pi}$, the solution of Eq. (6) has the form $\phi(\mathbf{r}) = \phi_0(\rho, z)/\sqrt{2\pi}$ and

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi} \sum_m e^{im(\varphi - \varphi')} G_m(\rho, z; \rho', z'), \quad F(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi} \sum_m e^{im(\varphi - \varphi')} F_m(\rho, z; \rho', z'). \quad (\text{B1})$$

The EOM for the wave function of coherent condensate reads

$$\partial_\tau \phi_0(\rho, z) = -\eta_0(\rho, z) - 2 \int \rho' d\rho' dz' [G_0(\rho, z; \rho', z') \eta_0(\rho', z') + F_0(\rho, z; \rho', z') \eta_0^*(\rho', z')], \quad (\text{B2})$$

where

$$\begin{aligned} \eta_0 &= h_0^{m=0} \phi_0(\rho, z) + \int \rho' d\rho' dz' U_0(\rho, z; \rho', z') [|\phi_0(\rho', z')|^2 + \sum_m G_m(\rho', z'; \rho', z')] \phi_0(\rho, z) \\ &\quad + \sum_m \int \rho' d\rho' dz' U_m(\rho, z; \rho', z') [G_m(\rho, z; \rho', z') \phi_0(\rho', z') + F_m(\rho, z; \rho', z') \phi_0^*(\rho', z')] + \eta_3 \end{aligned} \quad (\text{B3})$$

is determined by the contribution

$$\begin{aligned} \eta_3 = & \frac{g_3}{(2\pi)^2} \left\{ \frac{1}{2} |\phi_0(\rho, z)|^4 \phi_0(\rho, z) + \frac{1}{2} \sum_m F_m^*(\rho, z; \rho, z) \phi_0^3(\rho, z) + \frac{3}{2} \left| \sum_m F_m(\rho, z; \rho, z) \right|^2 \phi(\rho, z) \right. \\ & + 3 \sum_m G_m(\rho, z; \rho, z) [|\phi_0(\rho, z)|^2 + \sum_{m'} G_{m'}(\rho, z; \rho, z)] \phi_0(\rho, z) \\ & \left. + 3 \left[\frac{1}{2} |\phi_0(\rho, z)|^2 + \sum_m G_m(\rho, z; \rho, z) \right] \sum_{m'} F_{m'}(\rho, z; \rho, z) \phi_0^*(\rho, z) \right\} \end{aligned} \quad (\text{B4})$$

from the three-body interaction. The single-particle part

$$h_0^m = -\frac{1}{2M} \left(\partial_\rho^2 + \frac{1}{\rho} \partial_\rho - \frac{m^2}{\rho^2} \right) - \frac{1}{2M} \partial_z^2 + \frac{1}{2} M \omega_0^2 (\rho^2 + \lambda^2 z^2) - \mu \quad (\text{B5})$$

and the interaction

$$U_m(\rho, z; \rho', z') = \int \frac{d\varphi'}{2\pi} U(\mathbf{r} - \mathbf{r}') e^{-im(\varphi - \varphi')} \quad (\text{B6})$$

in the channel m will be treated carefully by the Hankel transformation, which can regularize the singularity in the dipolar interaction.

The EOM for the correlation functions are

$$\begin{aligned} \partial_\tau G_m(\rho, z; \rho', z') = & -[(\mathcal{E}G)_m + (\Delta F^\dagger)_m] - [(\mathcal{E}G)_m + (\Delta F^\dagger)_m]^\dagger \\ & - 2 \int \rho_1 d\rho_1 dz_1 \{ G_m(\rho, z; \rho_1, z_1) [(\mathcal{E}G)_m + (\Delta F^\dagger)_m](\rho_1, z_1; \rho', z') \\ & + F_m(\rho, z; \rho_1, z_1) [(\Delta G^T)_{-m}^* + (\mathcal{E}F)_{-m}^*](\rho_1, z_1; \rho', z') \} \end{aligned} \quad (\text{B7})$$

and

$$\begin{aligned} \partial_\tau F_m(\rho, z; \rho', z') = & -\Delta_3(\rho, z) \frac{1}{\rho} \delta(\rho - \rho') \delta(z - z') - \Delta_{\text{Bogo}}^m(\rho, z; \rho', z') \\ & - [(\mathcal{E}F)_m + (\Delta G^T)_m] - [(\Delta G^T)_{-m} + (\mathcal{E}F)_{-m}]^T \\ & - 2 \int \rho_1 d\rho_1 dz_1 \{ G_m(\rho, z; \rho_1, z_1) [(\mathcal{E}F)_m + (\Delta G^T)_m](\rho_1, z_1; \rho', z') \\ & + F_m(\rho, z; \rho_1, z_1) [(\Delta F^\dagger)_{-m}^* + (\mathcal{E}G)_{-m}^*](\rho_1, z_1; \rho', z') \}. \end{aligned} \quad (\text{B8})$$

Here, we use the short-hand notations

$$\begin{aligned} (\mathcal{E}G)_m(\rho, z; \rho', z') = & [h_0^m + \mathcal{E}_{\text{Hartree}}(\rho, z) + \mathcal{E}_3(\rho, z)] G_m(\rho, z; \rho', z') + \int \rho_1 d\rho_1 dz_1 \mathcal{E}_{\text{Fock}}^m(\rho, z; \rho_1, z_1) G_m(\rho_1, z_1; \rho', z'), \\ (\Delta F^\dagger)_m(\rho, z; \rho', z') = & \Delta_3(\rho, z) F_m^\dagger(\rho, z; \rho', z') + \int \rho_1 d\rho_1 dz_1 \Delta_{\text{Bogo}}^m(\rho, z; \rho_1, z_1) F_m^\dagger(\rho_1, z_1; \rho', z'), \end{aligned} \quad (\text{B9})$$

and

$$\begin{aligned} (\mathcal{E}F)_m(\rho, z; \rho', z') = & [h_0^m + \mathcal{E}_{\text{Hartree}}(\rho, z) + \mathcal{E}_3(\rho, z)] F_m(\rho, z; \rho', z') \\ & + \int \rho_1 d\rho_1 dz_1 \mathcal{E}_{\text{Fock}}^m(\rho, z; \rho_1, z_1) F_m(\rho_1, z_1; \rho', z'), \\ (\Delta G^T)_m(\rho, z; \rho', z') = & \Delta_3(\rho, z) G_{-m}^*(\rho, z; \rho', z') + \int \rho_1 d\rho_1 dz_1 \Delta_{\text{Bogo}}^m(\rho, z; \rho_1, z_1) G_{-m}^*(\rho_1, z_1; \rho', z'), \end{aligned} \quad (\text{B10})$$

which are determined by the Hartree-Fock-Bogoliubov terms

$$\begin{aligned} \mathcal{E}_{\text{Hartree}}(\rho, z) = & \int \rho_1 d\rho_1 dz_1 U_0(\rho, z; \rho_1, z_1) [|\phi_0(\rho_1, z_1)|^2 + \sum_{m'} G_{m'}(\rho_1, z_1; \rho_1, z_1)], \\ \mathcal{E}_{\text{Fock}}^m(\rho, z; \rho', z') = & \sum_{m'} U_{m-m'}(\rho, z; \rho', z') [\phi_0^*(\rho', z') \phi_0(\rho, z) \delta_{m'0} + G_{m'}(\rho, z; \rho', z')], \\ \Delta_{\text{Bogo}}^m(\rho, z; \rho', z') = & \sum_{m'} U_{m-m'}(\rho, z; \rho', z') [\phi_0(\rho', z') \phi_0(\rho, z) \delta_{m'0} + F_{m'}(\rho, z; \rho', z')], \end{aligned} \quad (\text{B11})$$

and the contribution

$$\begin{aligned}
\mathcal{E}_3(\rho, z) &= \frac{3}{2} \frac{g_3}{(2\pi)^2} \left\{ |\phi_0(\rho, z)|^4 + 4|\phi_0(\rho, z)|^2 \sum_{m'} G_{m'}(\rho, z; \rho, z) \right. \\
&\quad \left. + 2\text{Re}\phi_0^{*2}(\rho, z) \sum_{m'} F_{m'}(\rho, z, \rho, z) + 2 \left[\sum_{m'} G_{m'}(\rho, z; \rho, z) \right]^2 + \left| \sum_{m'} F_{m'}(\rho, z, \rho, z) \right|^2 \right\}, \\
\Delta_3(\rho, z) &= \frac{g_3}{(2\pi)^2} \left[|\phi_0(\rho, z)|^2 \phi_0^2(\rho, z) + 3\phi_0^2(\rho, z) \sum_{m'} G_{m'}(\rho, z; \rho, z) \right. \\
&\quad \left. + 3|\phi_0(\rho, z)|^2 \sum_{m'} F_{m'}(\rho, z, \rho, z) + 3 \sum_{m'm'_1} G_{m'}(\rho, z; \rho, z) F_{m'_1}(\rho, z, \rho, z) \right]
\end{aligned} \tag{B12}$$

from the three-body interactions.

APPENDIX C: COUPLED GP-LIKE EQUATIONS

In this section, we derive the coherent-squeezed state GPEs for condensates in the SBG phase by minimizing the ground-state energy E_0 . In the SBG phase, condensate wave function is characterized by a coherent mode and a squeezed mode, i.e., $\chi = (\phi_c, \phi_s)^T$, the correlation functions are approximated as

$$\langle \delta\psi^\dagger(\mathbf{r}') \delta\psi(\mathbf{r}) \rangle = \phi_s(\mathbf{r}) \phi_s^*(\mathbf{r}'), \quad \langle \delta\psi(\mathbf{r}') \delta\psi(\mathbf{r}) \rangle = \sqrt{1 + N_s^{-1}} \phi_s(\mathbf{r}) \phi_s(\mathbf{r}'), \tag{C1}$$

and the total energy E reads

$$E = \int d\mathbf{r} [\phi_c^*(\mathbf{r}) h_0 \phi_c(\mathbf{r}) + \phi_s^*(\mathbf{r}) h_0 \phi_s(\mathbf{r})] + E_{2B} + E_{3B}, \tag{C2}$$

where

$$\begin{aligned}
E_{2B} &= \int d\mathbf{r} d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \left[\frac{1}{2} |\phi_c(\mathbf{r})|^2 |\phi_c(\mathbf{r}')|^2 + |\phi_s(\mathbf{r})|^2 |\phi_c(\mathbf{r}')|^2 + \frac{1}{2} (3 + N_s^{-1}) |\phi_s(\mathbf{r})|^2 |\phi_s(\mathbf{r}')|^2 \right. \\
&\quad \left. + \phi_s^*(\mathbf{r}) \phi_s(\mathbf{r}') \phi_c^*(\mathbf{r}') \phi_c(\mathbf{r}) + \sqrt{1 + N_s^{-1}} \text{Re} \phi_s^*(\mathbf{r}) \phi_s^*(\mathbf{r}') \phi_c(\mathbf{r}') \phi_c(\mathbf{r}) \right],
\end{aligned} \tag{C3}$$

$$\begin{aligned}
E_{3B} &= g_3 \int d\mathbf{r} \left[\frac{1}{3!} |\phi_c|^6 + \frac{3}{2} (3 + N_s^{-1}) |\phi_c|^2 |\phi_s|^4 + \frac{1}{2} (5 + 3N_s^{-1}) |\phi_s|^6 \right. \\
&\quad \left. + \frac{3}{2} |\phi_c|^4 |\phi_s|^2 + \sqrt{1 + N_s^{-1}} \text{Re} |\phi_c|^2 \phi_c^2 \phi_s^{*2} + 3\sqrt{1 + N_s^{-1}} \text{Re} \phi_c^2 \phi_s^{*2} |\phi_s|^2 \right].
\end{aligned} \tag{C4}$$

The profiles of $\phi_{c,s}$ is determined by the imaginary time evolution $\partial_\tau \chi = -\delta E / \delta \chi^\dagger$. In the explicit form,

$$\begin{aligned}
\partial_\tau \phi_c(\mathbf{r}) &= -h_0 \phi_c(\mathbf{r}) - \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \{ [|\phi_c(\mathbf{r}')|^2 + |\phi_s(\mathbf{r}')|^2] \phi_c(\mathbf{r}) + [\phi_s^*(\mathbf{r}') \phi_c(\mathbf{r}') + \sqrt{1 + N_s^{-1}} \phi_c^*(\mathbf{r}') \phi_s(\mathbf{r}')] \phi_s(\mathbf{r}) \} \\
&\quad - \frac{1}{2} g_3 \{ [|\phi_c|^4 + 6|\phi_c|^2 |\phi_s|^2 + \sqrt{1 + N_s^{-1}} \phi_c^2 \phi_s^{*2} + 3(3 + N_s^{-1}) |\phi_s|^4] \phi_c + 3\sqrt{1 + N_s^{-1}} (|\phi_c|^2 \phi_s^2 + 2|\phi_s|^2 \phi_s^2) \phi_c^* \},
\end{aligned} \tag{C5}$$

and

$$\begin{aligned}
\partial_\tau \phi_s(\mathbf{r}) &= -h_0 \phi_s(\mathbf{r}) - \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \{ [|\phi_c(\mathbf{r}')|^2 + (3 + N_s^{-1}) |\phi_s(\mathbf{r}')|^2] \phi_s(\mathbf{r}) + [\phi_c^*(\mathbf{r}') \phi_s(\mathbf{r}') + \sqrt{1 + N_s^{-1}} \phi_s^*(\mathbf{r}') \phi_c(\mathbf{r}')] \phi_c(\mathbf{r}) \} \\
&\quad - \frac{1}{2} g_3 \{ [3|\phi_c|^4 + 6(3 + N_s^{-1}) |\phi_c|^2 |\phi_s|^2 + 3\sqrt{1 + N_s^{-1}} \phi_c^2 \phi_s^{*2} + 3(5 + 3N_s^{-1}) |\phi_s|^4] \phi_s \\
&\quad + \sqrt{1 + N_s^{-1}} (2|\phi_c|^2 \phi_c^2 + 9|\phi_s|^2 \phi_c^2) \phi_s^* \}.
\end{aligned} \tag{C6}$$

After some straightforward algebra, the above equations lead to Eqs. (21) in the main text.

FIG. 7. Density profiles $n_c(\rho, 0)$ (a), $n_c(0, z)$ (b), $n_s(\rho, 0)$ (c), $n_s(0, z)$ (d) for $N = 1400$ and $\varepsilon_{dd} = 1.38$ using GST (solid lines), 1.38 using cssGPE (dashed lines), 1.64 using GST (dotted lines), and 1.64 using cssGPE (dashed-dotted lines).

In Fig. 7, we compare the density profiles computed using the Gaussian-state theory and the effective equations derived here. To reveal more details, we plot the density profiles of the coherent and the squeezed components separately. As can be seen, for condensates in the SBG phase, the coherent-squeezed state GPE results agree with the full Gaussian-state theory very well when the parameters are away from the gas-liquid boundary.

APPENDIX D: APPENDIX D: WAVE FUNCTIONS IN THE SBL PHASE

In the SBL phase, the coherent component dominates in the condensates, which implies that the GPE should approx-

FIG. 8. Total density profiles along the radial direction (left) and along the z direction (right) are compared for wave functions obtained via the Gaussian-state theory and the GPE. The total number of atoms is $N = 1400$ and the relative dipolar interaction strengths are $\varepsilon_{dd} = 2.5$ and 1.77 for (a) and (b), and $\varepsilon_{dd} = 1.74$ and 1.64 for (c) and (d).

imately describe the system. In Fig. 8, we compare the total densities obtained via the Gaussian-state theory and the GPE under different ε_{dd} 's. It is apparent that the agreement between two approaches is improved as ε_{dd} grows, which demonstrates that, deep inside the SBL phase, the GPE with three-body repulsion can lead to the same results as those computed with the Gaussian-state theory.

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