

## Density-Functional Theory of Quantum Droplets

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In quantum droplets, the mean-field energy is comparable to the Lee-Huang-Yang (LHY) energy. In the Bogoliubov theory, the LHY energy of a quantum droplet has an imaginary part, which has been neglected in most studies for practical purposes. Thus far, most theoretical studies on quantum droplets have been based on the extended Gross-Pitaevskii (GP) equation, which includes the contribution of the LHY energy to the chemical potential. In this article, we present the density-functional theory of quantum droplets. In our approach, the quantum fluctuations in quantum droplets, as described by an effective action, generate a real correlation energy that can be determined consistently. Using density-functional theory, we calculated the energy, quantum depletion fraction, and excitations of the droplet. Our results for the ground-state energy and quantum depletion fractions were consistent with the Monte Carlo results. We also discuss the implications of our theory.

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*1. Introduction.* The creation of quantum droplets represents a breakthrough in the study of ultracold atoms in recent years. Quantum droplets have been experimentally realized in various systems, including dipolar Bose gases such as <sup>164</sup>Dy<sup>[1–5]</sup> and <sup>166</sup>Er<sup>[6]</sup> and binary boson mixtures such as homonuclear <sup>39</sup>K<sup>[7–9]</sup> and heteronuclear <sup>39</sup>K-<sup>87</sup>Rb mixtures.<sup>[10]</sup> In these experiments, quantum droplets were generated by tuning *s*-wave interactions using the Feshbach-resonance technique. Quantum droplets in binary dipolar mixtures have also been predicted.<sup>[11,12]</sup> In these quantum droplets, the mean-field energy is tuned to a weakly attractive energy, while the repulsive Lee-Huang-Yang (LHY) energy<sup>[13]</sup> arising from the quantum fluctuations becomes equally significant. The interplay between these two energies gives rise to a quantum-droplet state that is both self-bound and stable.

Due to the mean-field instability, the Bogoliubov theory, which describes Gaussian fluctuations around a uniform condensate, predicts imaginary excitation energies in the long-wavelength limit, indicating dynamical instability. Petrov<sup>[14]</sup> noted that these unstable excitations contribute minimally to the LHY energy and may become stabilized after renormalization by integrating out high-energy excitations. In practice, the LHY energy, with its imaginary component neglected, is widely applied in the extended Gross-Pitaevskii equation (EGPE)<sup>[14,15]</sup> to simulate quantum droplets. However, recent studies employing the Beliaev theory<sup>[16–18]</sup> have demonstrated that the dynamic instability predicted by the Bogoliubov theory is artificial. When higher-order quantum fluctuations are accounted for, the phonon energy becomes stable, as shown for both nondipolar Bose mixtures<sup>[16,17]</sup> and single-component dipolar Bose gases.<sup>[18]</sup>

In this paper, we present a density-functional theory of quantum droplets that self-consistently incorporates quantum fluctuations without encountering imaginary energies. The core of this method lies in accounting for the effects of higher-order fluctuations by renormalizing the *s*-wave coupling constants. For a binary boson mixture, the ground-state energies obtained using our approach show better agreement with the Monte Carlo (MC) simulation results<sup>[19]</sup> compared to those derived from the extended Gross-Pitaevskii equation (EGPE).<sup>[14]</sup> Similarly, for dipolar quantum droplets, our predictions for quantum depletion align more closely with MC results<sup>[20]</sup> than those based on Bogoliubov theory. Furthermore, we also discuss the implications of our theory.

*2. Density-Functional Approach.* We studied a multi-component Bose gas, with its Hamiltonian expressed as:

$$H = \int d\mathbf{r} \sum_{\sigma} \left[ \psi_{\sigma}^{\dagger}(\mathbf{r}) \left( -\frac{\hbar^2 \nabla^2}{2m_{\sigma}} + V_{\sigma}(\mathbf{r}) \right) \psi_{\sigma}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r}' \sum_{\sigma'} U_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}) \right], \quad (1)$$

where  $\psi_{\sigma}(\mathbf{r})$  is the boson field operator for the  $\sigma$  component,  $m_{\sigma}$  is the mass,  $V_{\sigma}(\mathbf{r})$  is the trap potential, and  $U_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}')$  represents the interaction between the bosons. For a BEC ground state, the condensate wavefunction is given by  $\psi_{0\sigma}(\mathbf{r}) = \langle \psi_{\sigma}(\mathbf{r}) \rangle = \sqrt{n_{0\sigma}(\mathbf{r})} e^{i\phi_{\sigma}(\mathbf{r})}$ , where  $n_{0\sigma}(\mathbf{r})$  denotes the condensate density and  $\phi_{\sigma}(\mathbf{r})$  denotes the condensate phase.

We considered the case where the temporal and spatial scales of the variances are significantly larger than the intrinsic scales of the system. Under these conditions, the

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local equilibrium assumption (LEA) can be applied, allowing the system to be described by the effective action:<sup>[21]</sup>

$$S_{\text{Eff}} = \int dt \int d\mathbf{r} \left\{ - \sum_{\sigma} n_{\sigma}(\mathbf{r}) [\hbar \partial_t \phi_{\sigma}(\mathbf{r}) + V_{\sigma}(\mathbf{r}) + \frac{\hbar^2}{2m_{\sigma}} \left( \frac{|\nabla n_{\sigma}(\mathbf{r})|^2}{4n_{\sigma}^2(\mathbf{r})} + |\nabla \phi_{\sigma}(\mathbf{r})|^2 \right) \right\} - \mathcal{E}_I(\mathbf{r}), \quad (2)$$

where  $n_{\sigma}(\mathbf{r})$  is the superfluid density, and  $\mathcal{E}_I$  is the interaction-energy density of the lowest-energy uniform state with the superfluid density  $n_{\sigma}$  and phase gradient  $\nabla \phi_{\sigma}$ . In the effective action  $S_{\text{Eff}}$ , there is no term involving the time derivative of the density.<sup>[22]</sup> From the effective action  $S_{\text{Eff}}$ , the superfluid hydrodynamic equations can be derived.<sup>[21]</sup> In the ground state, the superfluid phase is uniform,  $\phi_{\sigma} = 0$ , and, for simplicity, the interaction energy density  $\mathcal{E}_I$  can be expressed as the sum of two components:  $\mathcal{E}_I = \mathcal{E}_{\text{MF}} + \mathcal{E}_C$ , where the mean-field energy density is given by

$$\mathcal{E}_{\text{MF}}(\mathbf{r}) = \frac{1}{2} \int d\mathbf{r}' \sum_{\sigma, \sigma'} U_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') n_{\sigma}(\mathbf{r}) n_{\sigma'}(\mathbf{r}'). \quad (3)$$

The correlation energy density  $\mathcal{E}_C$ , as a function of densities, arises from quantum fluctuations beyond the mean field and should be determined self-consistently, as explained later in this section. The ground-state energy density,  $\mathcal{E}$ , is then given by  $\mathcal{E} = \mathcal{E}_K + \mathcal{E}_{\text{MF}} + \mathcal{E}_C$ , where the kinetic and potential energy densities are given by

$$\mathcal{E}_K(\mathbf{r}) = \sum_{\sigma} n_{\sigma}(\mathbf{r}) \left( \frac{\hbar^2}{2m_{\sigma}} \frac{|\nabla n_{\sigma}(\mathbf{r})|^2}{4n_{\sigma}^2(\mathbf{r})} + V_{\sigma}(\mathbf{r}) \right). \quad (4)$$

The superfluid-density distribution should satisfy the minimization condition of the ground-state energy,  $E = \int d\mathbf{r} \mathcal{E}$ :

$$- \frac{\hbar^2 \nabla^2 \sqrt{n_{\sigma}(\mathbf{r})}}{2m_{\sigma} \sqrt{n_{\sigma}(\mathbf{r})}} + V_{\sigma}(\mathbf{r}) + \int d\mathbf{r}' \sum_{\sigma'} U_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') n_{\sigma'}(\mathbf{r}') + \frac{\partial \mathcal{E}_C}{\partial n_{\sigma}} = \mu_{\sigma}, \quad (5)$$

where  $\mu_{\sigma} = \partial E / \partial N_{\sigma}$  is the chemical potential and  $N_{\sigma} = n_{\sigma} V$  is the boson number of the  $\sigma$  component. From Eq. (5), the density distribution of a nonuniform system can be determined in a manner analogous to solving the EGPE.

The central task is to calculate the correlation energy density  $\mathcal{E}_C$ . In the dilute region, a typical approach involves analyzing Gaussian fluctuations around the condensate and studying the Bogoliubov Hamiltonian. However, for systems such as quantum droplets, where beyond-mean-field effects play a critical role, this approach is insufficient, and the effects of higher-order fluctuations must be considered.<sup>[16–18]</sup> Here, we propose that for a uniform system, these significant fluctuation effects can be effectively captured through Gaussian fluctuations derived from the

effective action in Eq. (2), as expressed by:

$$S_2 = - \int dt \int d\mathbf{r} \sum_{\sigma} \left\{ \delta n_{\sigma}(\mathbf{r}) \hbar \partial_t \delta \phi_{\sigma}(\mathbf{r}) + \frac{\hbar^2}{2m_{\sigma}} \left( \left| \nabla \frac{\delta n_{\sigma}(\mathbf{r})}{4n_{\sigma}} \right|^2 + n_{\sigma} |\nabla \delta \phi_{\sigma}(\mathbf{r})|^2 \right) + \frac{1}{2} \int d\mathbf{r}' \sum_{\sigma'} U_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') \delta n_{\sigma}(\mathbf{r}) \delta n_{\sigma'}(\mathbf{r}') + \frac{1}{2} \sum_{\sigma'} \chi_{\sigma\sigma'}(\mathbf{r}) \delta n_{\sigma}(\mathbf{r}) \delta n_{\sigma'}(\mathbf{r}') \right\}, \quad (6)$$

where

$$\chi_{\sigma\sigma'} = \frac{\partial^2 \mathcal{E}_C}{\partial n_{\sigma} \partial n_{\sigma'}}. \quad (7)$$

For the homogeneous system under consideration, only the density and phase fluctuating fields,  $\delta n$  and  $\delta \phi$ , exhibit spatial dependence. Unlike the Bogoliubov theory, in Eq. (6), the Gaussian fluctuations refer to the density and phase fluctuations in the effective action, rather than the fluctuations around the condensate. This approach accounts for the crucial higher-order effects beyond the Bogoliubov theory. This renormalization of the Bogoliubov theory is equivalent to a local correction to the  $s$ -wave coupling constant, represented by  $\chi$  in Eq. (7). For a uniform system, the correlation energy can be determined by integrating out the fluctuating fields  $\delta n_{\sigma}$  and  $\delta \phi_{\sigma}$  in the action  $S_2$ , thus obtaining a self-consistent solution. Beyond the dilute region, higher-order fluctuations in the effective action should also be considered. In principle, the correlation energy density can still be derived by integrating out all fluctuating fields.

*3. Implications on Quantum Droplets.* Although the quantum droplets we studied are in the dilute region, the mean-field energy is very small and comparable to the LHY energy. Therefore, it is crucial to properly determine the correlation energy. In the following, we study the two types of quantum droplets observed in experiments: the binary boson mixture and the dipolar Bose gas.

*3.1. Binary Boson Mixture.* For a uniform binary boson mixture with short-range interactions, the action  $S_2$  in Eq. (6), which describes Gaussian fluctuations, is equivalent to a renormalized Bogoliubov Hamiltonian, given by

$$H_{\text{Eff}} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}, \sigma, \sigma'} g'_{\sigma\sigma'} \sqrt{n_{\sigma} n_{\sigma'}} \cdot \left[ a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma'} + \frac{1}{2} (a_{\mathbf{k}\sigma} a_{-\mathbf{k}\sigma'} + \text{H.C.}) \right], \quad (8)$$

where  $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ ,  $a_{\mathbf{k}\sigma}$  is the boson annihilation operator,  $g'_{\sigma\sigma'} = g_{\sigma\sigma'} + \chi_{\sigma\sigma'}$ , and  $g_{\sigma\sigma'}$  is the coupling constant between  $\sigma$ - and  $\sigma'$ -components. This effective Hamiltonian can first be written as the Hamiltonian of two independent single-species systems through a canonical transformation:

$$H_{\text{Eff}} = \sum_{\mathbf{k}, \lambda} \left[ (\epsilon_{\mathbf{k}} + \varepsilon_{\lambda}) b_{\mathbf{k}\lambda}^{\dagger} b_{\mathbf{k}\lambda} + \frac{1}{2} \varepsilon_{\lambda} (b_{\mathbf{k}\lambda} b_{-\mathbf{k}\lambda} + \text{H.C.}) \right], \quad (9)$$

where  $\varepsilon_{\pm}$  are eigenvalues of matrix  $M_{\sigma\sigma'} = g'_{\sigma\sigma'} \sqrt{n_{\sigma} n_{\sigma'}}$ ,

$$\varepsilon_{\pm} = \frac{1}{2} \left[ g'_{11} n_1 + g'_{22} n_2 \pm \sqrt{(g'_{11} n_1 - g'_{22} n_2)^2 + 4g'_{12}{}^2 n_1 n_2} \right],$$

$\lambda = \pm$ ,  $b_{\mathbf{k}\lambda} = \sum_{\sigma} u_{\lambda\sigma} a_{\mathbf{k}\sigma}$ , and  $u_{\lambda\sigma}$  is the normalized eigenvector of matrix  $M_{\sigma\sigma'}$ . From Eq. (9), two types of excitation can be obtained from this Hamiltonian: phonon and magnon,

$$E_{\mathbf{k}\lambda} = \sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2\epsilon_{\lambda})}. \quad (10)$$

Both energies exhibit linear dispersion in the long-wavelength limit, with the phonon speed  $c_-$  and the magnon speed  $c_+$

$$c_{\pm} = \sqrt{\frac{\epsilon_{\lambda}}{m}}. \quad (11)$$

In this case, the correlation energy corresponds to the renormalized LHY energy, as given by Ref. [23], and can be expressed in terms of these two speeds from Eq. (9), similar to the approach in the Bogoliubov theory:

$$\mathcal{E}_C = \frac{8m^4}{15\pi^2\hbar^3}(c_+^5 + c_-^5). \quad (12)$$

Speed  $c_{\pm}$  can be solved using Eqs. (12) and (7). For a dilute binary quantum droplet, where  $c_+ \gg c_-$  and  $|g_{\sigma\sigma'}| \gg |\chi_{\sigma\sigma'}|$ , the correlation energy, to leading order, is given by the LHY energy as presented in Ref. [14],

$$\mathcal{E}_C \approx \frac{\sqrt{2m^3}}{15\pi^2\hbar^3}(g_{11}n_1 + g_{22}n_2 + \sqrt{(g_{11}n_1 - g_{22}n_2)^2 + 4g_{12}^2n_1n_2})^{5/2}. \quad (13)$$

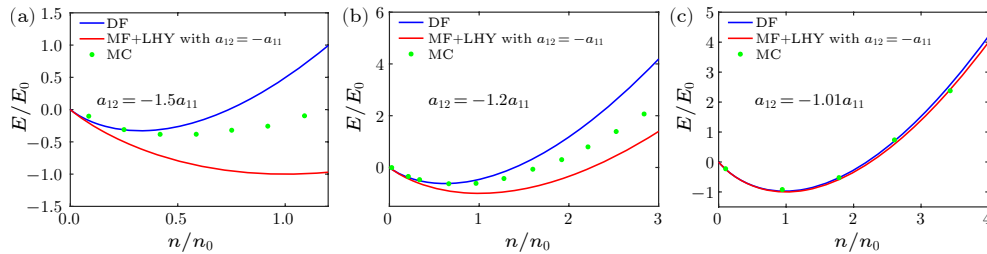
The second derivatives of  $\chi_{\sigma\sigma'}$  can be computed, yielding a positive phonon speed, in agreement with the results from

the Beliaev theory<sup>[16]</sup> and the path-integral approach.<sup>[17]</sup> This is also consistent with the results of Ref. [24], where the phonon speed was obtained from the hydrodynamical relation by considering only the real part of the LHY energy in the ground-state energy.

From Eq. (13), the equation of state for  $g_{22} = g_{11}$  is given by:

$$\begin{aligned} \frac{E}{N} &= \frac{(\mathcal{E}_{\text{MF}} + \mathcal{E}_C)V}{N} \\ &= \frac{\hbar^2\pi(a_{11} + a_{12})n}{m} + \frac{32\sqrt{2}\pi\hbar^2 a_{11}^{5/2}}{15m} \left(1 - \frac{a_{12}}{a_{11}}\right)^{\frac{5}{2}} n^{\frac{3}{2}}, \end{aligned} \quad (14)$$

where  $a_{\sigma\sigma'} = \frac{mg_{\sigma\sigma'}}{4\pi\hbar^2}$  is the  $s$ -wave scattering length,  $n = N/V$  is the density, and  $N$  is the total particle number. In Fig. 1, we present the results obtained using Eq. (14) for different values of the interspecies scattering length  $a_{12}$  and compare them with the Monte Carlo (MC) equations of state<sup>[19]</sup> and the MF+LHY prediction.<sup>[14]</sup> In Ref. [14], to avoid the existence of imaginary parts in the LHY energy,  $|a_{12}|$  is approximated as  $a_{11}$ . The density-functional equations of state from Eq. (14) do not contain imaginary parts and are in close agreement with the MC results, particularly in the region where the density is lower than the equilibrium density. When  $|a_{12}|$  deviates from  $a_{11}$ , for  $na_{11}^3 < 2 \times 10^{-4}$ , our results agree well with the MC results, as shown in Figs. 1(a) and 1(b). At larger densities, our results start to deviate from the MC data, probably due to the higher-order effects neglected in our approach.



**Fig. 1.** For the binary boson mixture droplet,<sup>[19]</sup> we compared the equations of state predicted by our density-functional theory, the MF+LHY approximation with  $|a_{12}| = a_{11}$ ,<sup>[14]</sup> and MC results for different values of the interspecies scattering length  $a_{12}$ . The green dots represent the MC results,<sup>[19]</sup> the blue line shows our results from Eq. (14), and the red line depicts the MF+LHY prediction with  $|a_{12}| = a_{11}$ , as done in Ref. [14]. The definitions of energy units  $E_0$  and density units  $n_0$  are consistent with those used in Ref. [19].

The equation of state for the pairing state also showed good agreement with the MC results.<sup>[25–28]</sup> There are crucial differences in the excitation spectra between the BEC state and the pairing state, which can be used to determine the true ground state. In the BEC state of a binary mixture, both phonon and magnon excitations are gapless. In contrast, in the pairing state, the magnon excitation is gapped, while the phonon mode remains gapless. Some higher-order corrections can also be obtained by utilizing the thermodynamic relation for compressibility, while ignoring the imaginary components in the compressibility and energy due to fluctuations in the density channel.<sup>[24]</sup> In contrast, within the framework of the density-functional theory, both density and phase fluctuations are treated

self-consistently, and the correlation energy can be obtained without the problem of imaginary components in the LHY energy.

**3.2. Dipolar Bose Gas.** For a dilute uniform dipolar Bose gas with all dipoles aligned along the  $z$ -direction, the renormalized Bogoliubov Hamiltonian corresponding to the quadratic action  $S_2$  is given by

$$H_{\text{Eff}} = \sum_{\mathbf{k}} \left[ (\epsilon_{\mathbf{k}} + U'(\mathbf{k})n) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} U'(\mathbf{k})n (a_{\mathbf{k}} a_{-\mathbf{k}} + \text{H.C.}) \right], \quad (15)$$

where  $U'(\mathbf{k}) = U(\mathbf{k}) + \chi$ ,  $U(\mathbf{k}) = g[1 + \epsilon_{dd}(3\cos^2\phi_{\mathbf{k}} - 1)]$ ,  $g$  is the  $s$ -wave coupling constant,  $\epsilon_{dd}$  is the strength of the dipole-dipole interaction, and  $\phi_{\mathbf{k}}$  is the angle between

$\mathbf{k}$  and the  $z$ -axis. The correlation energy is given by<sup>[29,30]</sup>

$$\mathcal{E}_C = \frac{64}{15\sqrt{\pi}} g' n^2 \sqrt{na^3} Q_5(\epsilon'_{dd}), \quad (16)$$

where  $g' = g + \chi$ ,  $\epsilon'_{dd} = g\epsilon_{dd}/g'$ ,  $a' = mg'/(4\pi\hbar^2)$ ,

$$Q_5(x) = \frac{(3x)^{5/2}}{48} \left[ (8 + 26y + 33y^2) \sqrt{1+y} + 15y^3 \ln \frac{1+\sqrt{1+y}}{\sqrt{y}} \right],$$

and  $y = (1-x)/3x$ .  $\chi$  as a function of the density can be solved self-consistently using Eq. (16) and (17). In the dilute limit,  $g' \approx g$ , the correlation energy is given by the LHY energy:

$$\mathcal{E}_C \approx \frac{64}{15\sqrt{\pi}} gn^2 \sqrt{na^3} Q_5(\epsilon_{dd}), \quad (17)$$

where  $a = mg/(4\pi\hbar^2)$ . The effective correction to the  $s$ -wave coupling constant is approximately given by:

$$\chi \approx \frac{16}{\sqrt{\pi}} g \sqrt{na^3} Q_5(\epsilon_{dd}), \quad (18)$$

as found in Ref. [18].

For a quantum droplet, where  $\epsilon_{dd} > 1$ , the function  $Q_5(\epsilon_{dd})$  has a small imaginary part, which is neglected in the EGPE.<sup>[15,31]</sup> However, in our approach, the imaginary energy problem is avoided from the outset. From Eq. (16), we obtain:

$$\frac{d\mathcal{E}_C}{dn} = \frac{32}{3\sqrt{\pi}} g' \sqrt{na^3} Q_5(\epsilon'_{dd}) + \frac{64}{15\sqrt{\pi}} g' n^2 \sqrt{na^3} \cdot \left[ \frac{5}{2g'} \frac{dg'}{dn} Q_5(\epsilon'_{dd}) + Q'_5(\epsilon'_{dd}) \frac{d\epsilon'_{dd}}{dn} \right], \quad (19)$$

where  $Q'_5(x) = dQ_5(x)/dx$ . In the dilute region, the density dependence of  $g'$  and  $\epsilon'_{dd}$  is weak, and Eq. (19) can be approximated as

$$\frac{d\mathcal{E}_C}{dn} \approx \frac{32}{3\sqrt{\pi}} gn \sqrt{na^3} Q_5(\epsilon'_{dd}). \quad (20)$$

Similarly, from Eq. (7), the correction to the  $s$ -wave coupling constant is approximately given by

$$\chi = \frac{d^2\mathcal{E}_C}{dn^2} \approx \frac{16}{\sqrt{\pi}} g \sqrt{na^3} Q_5(\epsilon'_{dd}). \quad (21)$$

Thus, the renormalized  $s$ -wave coupling constant  $g'$  can be obtained self-consistently as follows:

$$g' = g + \frac{16}{\sqrt{\pi}} g \sqrt{na^3} Q_5(\epsilon'_{dd}). \quad (22)$$

As described in Ref. [18], the renormalized parameter  $\epsilon'_{dd}$  is less than one, and the imaginary-energy problem is artificial. Here, we verify the accuracy of this approximation by computing the quantum depletion fraction and comparing it with the MC results.<sup>[20]</sup> For a uniform dipolar Bose gas with density  $n$ , in Bogoliubov theory, the quantum depletion fraction is given by:<sup>[30]</sup>

$$f_d^B = \frac{8}{3} \sqrt{na^3/\pi} Q_3(\epsilon_{dd}), \quad (23)$$

where

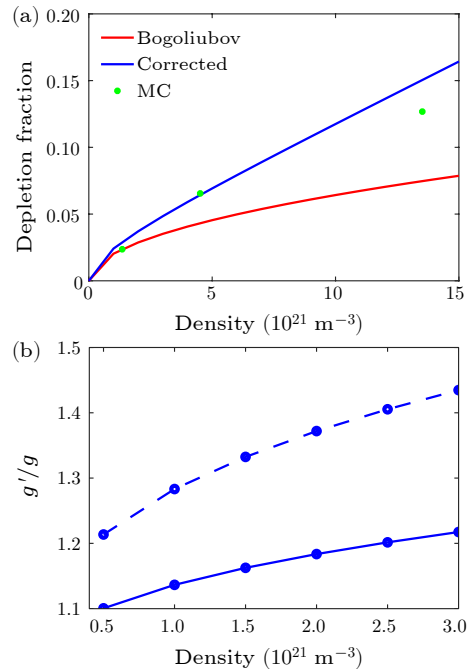
$$Q_3(x) = \frac{(3x)^{3/2}}{8} \left[ (2 + 5y) \sqrt{1+y} + 3y^2 \ln \frac{1+\sqrt{1+y}}{\sqrt{y}} \right],$$

$$y = \frac{(1-x)}{3x}.$$

Using the renormalized  $s$ -wave coupling constant  $g'$ , we obtain the corrected quantum depletion fraction as

$$f_d^c = \frac{8}{3} \sqrt{na^3/\pi} Q_3(\epsilon'_{dd}). \quad (24)$$

In Fig. 2(a), we compare the corrected depletion fraction  $f_d^c$  with those from the MC calculation results<sup>[20]</sup> and the Bogoliubov theory. Our results are consistent with the MC results, particularly in the region with a larger quantum depletion fraction, and both deviate from the Bogoliubov theory as the density increases. This suggests that dipolar quantum droplets have stronger quantum fluctuations than those described by the Gaussian fluctuations in the Bogoliubov theory.



**Fig. 2.** For the uniform system with parameters from the  $^{162}\text{Dy}$  droplet,<sup>[20]</sup> (a) the depletion fraction as predicted by our density-functional theory, MC results, and the Bogoliubov theory, for a scattering length of  $a = 60a_0$ . The green dots represent the MC results,<sup>[20]</sup> the blue line shows our results obtained using Eq. (24), and the red line shows the Bogoliubov theory results from Eq. (23). (b)  $g'/g$  as a function of the density for  $\epsilon_{dd} = 1.2$ ,  $a = 107.5a_0$  (dashed line) and  $a = 60a_0$  (solid line).

For dipolar Bose gases, the excitation energy in Bogoliubov theory is given by

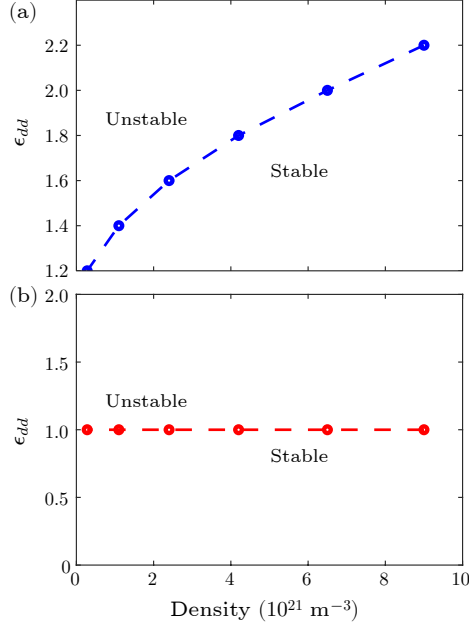
$$\epsilon_B = \sqrt{\epsilon_k(2nU(\mathbf{k}) + \epsilon_k)}. \quad (25)$$

In the quantum-droplet region, where the strength of the dipole-dipole interaction  $\epsilon_{dd} > 1$ , there is an imaginary part in the excitation energy for  $\phi_{\mathbf{k}} = \pi/2$ , implying dynamical instability. In our density-functional theory, the renormalized strength of the dipole-dipole interaction  $\epsilon'_{dd}$

can still be less than one, thereby stabilizing the excitation spectrum, which is given by

$$\epsilon'_B = \sqrt{\epsilon_k(2nU'(\mathbf{k}) + \epsilon_k)}. \quad (26)$$

In Fig. 3, we show the stable region of the renormalized excitation spectrum for different droplet densities and  $\epsilon_{dd}$ .



**Fig. 3.** For the uniform system with parameters from the  $^{162}\text{Dy}$  droplet,<sup>[20]</sup> the blue line in (a) shows the stable boundary of the excitation spectrum predicted by our density-functional theory, and the red line in (b) shows the stable boundary of the excitation spectrum predicted by Bogoliubov theory.

In the experiments, the systems are non-uniform with finite sizes. The dynamical instability occurs when the ground state becomes degenerate with the first excitation state.<sup>[32]</sup> Nonetheless, the energy density of a uniform system is important for the theoretical treatment of non-uniform systems, such as in the EGPE and a recent MC

$$I_{\pm\sigma\sigma'}(\mathbf{k}) = \frac{\partial I_{\pm\sigma}(\mathbf{k})}{\partial n_{\sigma'}} \approx \mp \left\{ \frac{[(-1)^{\bar{\sigma}} \Delta(\mathbf{k}) U'_{\sigma\sigma}(\mathbf{k}) + 2n_{\bar{\sigma}} U'_{12}{}^2(\mathbf{k})] (-1)^{\bar{\sigma}'} \Delta(\mathbf{k}) U'_{\sigma'\sigma'}(\mathbf{k}) + 2n_{\bar{\sigma}'} U'_{12}{}^2(\mathbf{k})}{[\Delta^2(\mathbf{k}) + 4n_1 n_2 U'_{12}{}^2(\mathbf{k})]^{3/2}} - \frac{(-1)^{\bar{\sigma}+\bar{\sigma}'} U'_{\sigma'\sigma'}(\mathbf{k}) U'_{\sigma\sigma}(\mathbf{k}) + 2\delta_{\sigma'\bar{\sigma}} U'_{12}{}^2(\mathbf{k})}{\sqrt{\Delta^2(\mathbf{k}) + 4n_1 n_2 U'_{12}{}^2(\mathbf{k})}} \right\}, \quad (32)$$

$\bar{\sigma}$  labels the component different from  $\sigma$ ,  $\bar{1} = 2$ ,  $\bar{2} = 1$ . As done previously, the density dependence of  $g'_{\sigma\sigma'}$  is neglected. From Eq. (30), the correction to the  $s$ -wave coupling constant  $\chi_{\sigma\sigma'}$  can be solved, and other renormalized physical quantities can be obtained thereafter.

4. *Discussion.* It is worth mentioning that density functional theory was used to study  $^4\text{He}$  droplets<sup>[34]</sup>, where the interaction parameters were treated phenomenologically. In the density functional theory of quantum droplets, quantum fluctuations renormalize  $s$ -wave coupling constants, which can be determined self-consistently in the dilute region. The results from our approach are consistent with those of the EGPE but do not suffer from

study based on density functional theory.<sup>[33]</sup>

Our approach can also be extended to a dilute binary dipolar Bose gas, with an effective quadratic Hamiltonian given by

$$H_{\text{Eff}} = \sum_{\mathbf{k}\sigma} \epsilon_k a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma,\sigma'} U'_{\sigma\sigma'}(\mathbf{k}) \sqrt{n_\sigma n_{\sigma'}} \cdot \left[ a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma'} + \frac{1}{2} (a_{\mathbf{k}\sigma} a_{-\mathbf{k}\sigma'} + \text{H.C.}) \right], \quad (27)$$

where  $U'_{\sigma\sigma'}(\mathbf{k}) = U_{\sigma\sigma'}(\mathbf{k}) + \chi_{\sigma\sigma'}$ ,  $U_{\sigma\sigma'}(\mathbf{k}) = g_{\sigma\sigma'}^s + g_{\sigma\sigma'}^d(3\cos^2\phi_{\mathbf{k}} - 1)$ ,  $g_{\sigma\sigma'}^s$  and  $g_{\sigma\sigma'}^d$  are the coupling constants of the  $s$ -wave and dipolar interactions. In a uniform state, the correlation energy can be obtained from this effective Hamiltonian in the same manner as described in Ref. [12], except that there is now a correction,  $\chi_{\sigma\sigma'}$ , to the  $s$ -wave coupling constant, which can be determined self-consistently as shown in Eq. (7). The correlation energy density is given by<sup>[12]</sup>

$$\epsilon_C = \frac{\sqrt{2}m^{3/2}}{15\pi^2\hbar^3} \sum_{\pm} \int_0^{\pi/2} d\theta_k \sin\theta_k I_{\pm}^{5/2}(\mathbf{k}), \quad (28)$$

where

$$I_{\pm}(\mathbf{k}) = n_1 U'_{11}(\mathbf{k}) + n_2 U'_{22}(\mathbf{k}) \pm \sqrt{\Delta^2(\mathbf{k}) + 4n_1 n_2 U'_{12}{}^2(\mathbf{k})}, \quad (29)$$

$\Delta(\mathbf{k}) = n_1 U'_{11}(\mathbf{k}) - n_2 U'_{22}(\mathbf{k})$ . Thus, the correction to the  $s$ -wave coupling constant can be obtained as:

$$\chi_{\sigma\sigma'} = \frac{\sqrt{2}m^{3/2}}{6\pi^2\hbar^3} \sum_{\pm} \int_0^{\pi/2} d\theta_k \sin\theta_k \cdot I_{\pm}^{1/2}(\mathbf{k}) \left[ \frac{3}{2} I_{\pm\sigma}(\mathbf{k}) I_{\pm\sigma'}(\mathbf{k}) + I_{\pm}(\mathbf{k}) I_{\pm\sigma\sigma'}(\mathbf{k}) \right], \quad (30)$$

where

$$I_{\pm\sigma}(\mathbf{k}) = \frac{\partial I_{\pm}(\mathbf{k})}{\partial n_\sigma} \approx U'_{\sigma\sigma}(\mathbf{k}) \pm \frac{(-1)^{\bar{\sigma}} \Delta(\mathbf{k}) U'_{\sigma\sigma}(\mathbf{k}) + 2n_{\bar{\sigma}} U'_{12}{}^2(\mathbf{k})}{\sqrt{\Delta^2(\mathbf{k}) + 4n_1 n_2 U'_{12}{}^2(\mathbf{k})}}, \quad (31)$$

the imaginary-energy problem. Our results for the ground-state energy and the quantum depletion fractions agree with the MC results. For systems with significant quantum depletion, our approach should be superior because it treats quantum fluctuations self-consistently.

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