Microscopic pairing theory of ultradilute low-dimensional quantum droplets

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Ultradilute quantum droplets are intriguing new state of matter, in which the attractive mean-field force can be balanced by the repulsive force from quantum fluctuations to avoid collapse. Here, we present a microscopic theory of ultradilute quantum droplets in low-dimensional two-component Bose-Bose mixtures, by generalizing the conventional Bogoliubov theory to include the bosonic pairing arising from the inter-species attraction. Our pairing theory is fully equivalent to a variational approach and hence gives an upper bound for the energy of quantum droplets. In one dimension, we find that the energy calculated by the pairing theory is in an excellent agreement with the latest diffusion Monte Carlo simulation [Phys. Rev. Lett. 122, 105302 (2019)], for nearly all the interaction strengths at which quantum droplets exist. In two dimensions, we show that quantum droplets disappear and may turn into a soliton-like many-body bound state, when the inter-species attraction exceeds a critical value. Below the threshold, the pairing theory predicts more or less the same results as the Bogoliubov theory derived by Petrov and Astrakharchik [Phys. Rev. Lett. 117, 100401 (2016)]. The predicted energies from both theories are higher than the diffusion Monte Carlo results, due to the weak inter-species attraction and the increasingly important role played by the beyond-Bogoliubov-approximation effect in two dimensions. Our pairing theory provides an ideal starting point to understand interesting ground-state properties of quantum droplets, including their shape and collective oscillations.

I. INTRODUCTION

In the weakly interacting regime, quantum phase of ultracold atomic Bose gases is typically determined by their mean-field interactions [1]. Attractive mean-field interactions can induce mechanical instability towards collapse [2]. This common viewpoint, however, is radically changed due to the seminal work by Petrov [3], who proposed that the mean-field collapse could be prevented by the repulsive force provided by quantum fluctuations, i.e., the celebrated Lee-Huang-Yang (LHY) correction to the energy functional [4]. Although the beyond-mean-field LHY correction is usually small, it can be made comparable to the mean-field energy by experimentally tuning the interatomic interactions with the Feshbach resonance technique. As a result, self-bound liquid-like quantum droplets may form, even in free space without container [5–7]. Petrov’s ground-breaking proposal has now been surprisingly confirmed in single-component Bose gases with anisotropic dipolar forces [8–12] and in two-component Bose-Bose mixtures with contact inter-particle interactions [13–17]. It opens a new rapidly developing research field, where the beyond-mean-field many-body effect could be systematically explored, both experimentally [8–12] and theoretically [13–32].

Despite the great success of Petrov’s proposal, strictly speaking, it is not a consistent microscopic theory. This is particularly clear for three-dimensional Bose-Bose mixtures, with which the Petrov prototype theory of quantum droplets was constructed, within the Bogoliubov approximation [3,35]. As the mean-field solution is not stable towards collapse, one of the two gapless Bogoliubov modes becomes softened and acquires a small imaginary component. This results in a complex LHY energy functional [3,28,33,34], which is not physical. To circumvent this technical issue, Petrov assumed a weak dependence of the LHY energy functional on the inter-species interaction strength and fixed the LHY energy to the value on the verge of the collapse where the mechanical instability first sets in [3]. Hereafter, we will refer to such an approximation as Petrov’s prescription. Due to the intrinsic inconsistency in the Petrov prototype theory, the resulting energy of quantum droplets shows an appreciable deviation from the numerically accurate diffusion Monte Carlo (DMC) predictions [28]. The predicted critical number for the droplet formation also seems to be larger than the one measured experimentally, both in dipolar Bose gases [11] and in Bose-Bose mixtures [13].

Recently, we developed a consistent microscopic theory to remove the annoying loophole in the Petrov theory of quantum droplets [33]. The crucial ingredient of the theory is the inclusion of the bosonic pairing between different components due to the attractive inter-species interactions. The pairing explicitly removes the unstable softened Bogoliubov excitation and turns it into a stable gapped mode, as in the conventional Bardeen-Cooper-Schrieffer theory for interacting fermions [36]. An apparent advantage of the pairing theory is that, it is variational and therefore predicts an upper bound for the ground-state energy. Remarkably, in three dimensions our pairing theory leads to an improved agreement with the DMC simulation, for the energy and the equilibrium density of quantum droplets [33].

In this work, we would like to provide more details of the microscopic pairing theory in three dimensions [33], on the equation derivation, the numerical calculation and the comparison to the DMC results [28]. We then focus on the new cases of low-dimensional quantum droplets and examine systematically their bulk properties. Our pairing theory turns out to work extremely well in one
dimension. For nearly all the interaction strengths at which quantum droplets exist, we find an excellent agreement between the theory and the DMC simulation for the ground-state energy \[27\]. In two dimensions, quantum droplets emerge for an arbitrarily weak inter-species interaction strength. Due to the weakness of the inter-species attraction, our pairing theory does not differ too much with the Petrov theory \[13\]. Both theories fail to have a good agreement with the DMC simulation, presumably due to the beyond-LHY-correction that becomes increasingly important in two dimensions \[27, 38\]. Nevertheless, it is remarkable that with increasing inter-species attraction our pairing theory predicts a critical attraction, above which quantum droplets cease to exist. This critical value is consistent with the threshold for zero-crossing in dimer-dimer scatterings from a four-body problem in two dimensions \[39\]. Above the threshold, the effective interaction between dimers (i.e., tightly bound bosonic pairs) changes from weakly attractive to weakly repulsive, indicating the instability of quantum droplets in the few-body limit.

The rest of the paper is organized as follows. In the next section (Sec. II), we introduce the model Hamiltonian for two-component Bose-Bose mixtures and present the pairing theory, i.e., the Bogoliubov theory with bosonic pairing. In Sec. III, the connection of our pairing theory to the conventional Bogoliubov theory without pairing is discussed. In Sec. IV, Sec. V, and Sec. VI, we consider the three-, one-, and two-dimensional cases, respectively. In each case, we discuss in detail the comparison of the pairing theory to the benchmark DMC simulations. Finally, Sec. VII is devoted to conclusions.

II. THE MODEL HAMILTONIAN AND PAIRING THEORY

We consider a two-component Bose-Bose mixture as in the seminal work by Petrov \[8\]. To be specific, let us focus on homonuclear mixtures such as the \(^{39}\)K-\(^{39}\)K mixture, with which the masses of the two components are the same, i.e., \(m_1 = m_2 = m\). In the presence of the intra-species interactions \(g_{11}\) and \(g_{22}\), and the interspecies interactions \(g_{12} = g_{21}\), the system in free space can be described by the following model Hamiltonian density,

\[
\mathcal{H}(x) = \mathcal{H}_0(x) + \mathcal{H}_{\text{int}}(x),
\]

\[
\mathcal{H}_0(x) = \sum_{i=1,2} \phi_i^\dagger(x) \left[ -\frac{\hbar^2 \nabla^2}{2m} - \mu_i \right] \phi_i(x),
\]

\[
\mathcal{H}_{\text{int}}(x) = \sum_{i,j=1,2} \frac{g_{ij}}{2} \phi_i^\dagger(x) \phi_j^\dagger(x) \phi_j(x) \phi_i(x),
\]

where \(\phi_i(x) (i = 1, 2)\) is the annihilation field operator of the \(i\)-species bosons and \(\mu_i\) is the chemical potential. In three or two dimensions, the use of contact inter-particle interactions leads to the well-known ultraviolet divergence, so the bare interaction strengths \(g_{ij}\) need regularization and are to be replaced by the \(s\)-wave scattering lengths \(a_{ij}\) or the binding energies \(E_{ij}^s\). For example, in three dimensions we may write,

\[
\frac{1}{g_{ij}} = \frac{m}{4\pi \hbar^2 a_{ij}} - \frac{1}{V} \sum_k \frac{m}{\hbar^2 k^2},
\]

where the volume \(V\) (or area in two dimensions and length in one dimension) will be set to unity hereafter.

We use the conventional path-integral formalism to describe our bosonic pairing theory, following its fermionic counterpart \[10, 11\]. We are interested in calculating the thermodynamic potential \(\Omega\) from the partition function,

\[
\mathcal{Z} = \int \mathcal{D}[\phi_1, \phi_2] e^{-\mathcal{S}},
\]

where the action is given by,

\[
\mathcal{S} = \int dx \left[ \sum_{i=1,2} \bar{\phi}_i(x) \partial_t \phi_i(x) + \mathcal{H}(x) \right].
\]

Here, we have used the standard notations \(x \equiv (x, \tau)\) and \(\int dx \equiv \int dx \int_0^\beta d\tau\), and \(\beta \equiv 1/(k_B T)\).

Due to the attractive interspecies interaction (i.e, \(g_{12} < 0\)), we anticipate the pairing between different species. To make it evident, we explicitly introduce an auxiliary pairing field \(\Delta(x)\) and take the Hubbard–Stratonovich transformation to decouple the Hamiltonian density for inter-species interactions, i.e.,

\[
\exp \left[ -g_{12} \int dx \bar{\phi}_1 \phi_2 \phi_1^\dagger \phi_2^\dagger \right] = \int \mathcal{D}[\Delta(x)] \exp \left\{ \int dx \left[ \frac{|\Delta(x)|^2}{g_{12}} + (\bar{\Delta} \phi_2 \phi_1 + \phi_1^\dagger \phi_2^\dagger \Delta) \right] \right\}. \tag{6}
\]

The action then becomes,

\[
\mathcal{S} = \int dx \left[ -\frac{|\Delta(x)|^2}{g_{12}} - (\bar{\Delta} \phi_2 \phi_1 + \phi_1^\dagger \phi_2^\dagger \Delta) \right] + \sum_{i=1,2} \int dx \left[ \bar{\phi}_i \left( \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu_i \right) \phi_i + \frac{g_{ii}}{2} \bar{\phi}_i^\dagger \phi_i^\dagger \phi_i \phi_i \right]. \tag{7}
\]

For the pairing field \(\Delta(x)\), it suffices to take a uniform saddle-point solution \(\Delta(x) = \Delta > 0\). At the same level of the Bogoliubov approximation, at zero temperature we assume the bosons condensate into the zero-momentum
states, i.e.,
\[ \phi_i (x) = \phi_{ic} + \delta \phi_i (x), \quad (8) \]

with a positive wave-function \( \phi_{ic} > 0 \). Following the Bogoliubov approximation, the intra-species interaction terms may be approximated as,
\[ \frac{g_{ii}}{2} \phi_i^2 \phi_j^2 \simeq C_i^2 + \frac{C_i}{2} \left( 4 \phi_i \delta \phi_i + \phi_j \delta \phi_j + \delta \phi_i \delta \phi_j \right), \quad (9) \]

where \( C_i = g_{ii} \phi_{ic}^2 \). As a consequence, we find the effective action \( S \simeq \beta V \Omega_0 + S_B \), where the condensate thermodynamic potential \( \Omega_0 \) is given by,
\[ \Omega_0 = \sum_{i=1,2} \left( -\mu_i \phi_{ic}^2 + \frac{C_i^2}{2g_{ii}} \right) - \frac{\Delta^2}{g_{12}} - 2 \Delta \phi_{ic} \phi_{2c}, \quad (10) \]

and the quantum fluctuations around the condensates have the contribution,
\[ S_B = - \int dx \Delta \left( \hat{\delta} \phi_1 \delta \phi_2 + \delta \phi_2 ^2 \phi_1 \right) + \int dx \sum_{i=1,2} \left[ \delta \phi_i \left( \hat{B}_i + \hat{\bar{B}}_i \right) \delta \phi_i + \frac{C_i}{2} \left( \delta \phi_i \delta \bar{\phi}_i + \delta \bar{\phi}_i \delta \phi_i \right) \right], \quad (11) \]

with \( \hat{B}_i (x) \equiv - \hbar^2 \nabla^2 / (2m) - \mu_i + 2C_i \). By introducing a Nambu spinor \( \Phi(x) = [\delta \phi_1(x), \delta \phi_1(x), \delta \phi_2(x), \delta \bar{\phi}_2(x)]^T \),

we obtain the two Bogoliubov spectra,
\[ E_{\pm}^2 (k) = \left[ A_+ (k) - \Delta^2 \right] \pm \sqrt{A_-^2 (k) + \Delta^2 \left[ (C_1 + C_2)^2 - (B_{1k} - B_{2k})^2 \right]}, \quad (17) \]

where we have defined,
\[ A_+ (k) = \frac{(B_{1k}^2 - C_1^2) \pm (B_{2k}^2 - C_2^2)}{2}. \quad (18) \]

A. Thermodynamic potential

By taking the derivative of the condensate thermodynamic potential \( \Omega_0 \) in Eq. (10) with respect to \( \phi_{ic} \) and \( \phi_{2c} \), we find that,
\[ -\mu_1 \phi_{ic} + g_{11} \phi_{ic}^3 - \Delta \phi_{2c} = 0, \quad (19) \]
\[ -\mu_2 \phi_{2c} + g_{22} \phi_{2c}^3 - \Delta \phi_{1c} = 0. \quad (20) \]

Therefore, we obtain
\[ -\mu_1 + C_1 = B_{1k=0} - C_1 = \Delta \left( \phi_{2c}/\phi_{1c} \right), \quad (21) \]
\[ -\mu_2 + C_2 = B_{2k=0} - C_2 = \Delta \left( \phi_{1c}/\phi_{2c} \right). \quad (22) \]

we may recast \( S_B \) into a compact form,
\[ S_B = \int dx dx' \Phi(x) \left[ -\partial^{-1} (x, x') \right] \Phi(x'), \quad (12) \]

where the inverse Green function of bosons is given by,
\[ \partial^{-1} = \begin{pmatrix} -\partial_x - \hat{B}_1 & -C_1 & 0 & \Delta \\ -C_1 & \partial_x - \hat{\bar{B}}_1 & \Delta & 0 \\ 0 & \Delta & -\partial_x - \hat{B}_2 & -C_2 \\ \Delta & 0 & -C_2 & \partial_x - \hat{\bar{B}}_2 \end{pmatrix}. \quad (13) \]

Due to the delta function \( \delta (x - x') \) in \( \partial^{-1} (x, x') \), which we do not explicitly show in the above equation, it is convenient to work in momentum space by performing a Fourier transform. After replacing \( -\partial_x \) with the bosonic Matsubara frequencies \( i \omega_m \) (i.e., \( \omega_m = 2 \pi m k_B T \) with \( m \in \mathbb{Z} \)) and performing the analytic continuation \( i \omega_m \rightarrow \omega + i0^+ \), i.e.,
\[ -\partial_x \rightarrow \omega + i0^+, \quad (14) \]

and taking the replacement
\[ \hat{B}_i \rightarrow B_{ik} = \epsilon_k - \mu_i + 2C_i \quad (15) \]

with \( \epsilon_k = \hbar^2 k^2 / (2m) \), it is straightforward to explicitly write down the expression of \( \partial^{-1} (k, \omega) \). By solving the poles of the bosonic Green function, i.e., \( \det [\partial^{-1} (k, \omega)] = 0 \), or more explicitly,
\[ \omega^4 - \omega^2 \left[ (B_{1k}^2 - C_1^2) + (B_{2k}^2 - C_2^2) - 2 \Delta^2 \right] + \left[ (B_{1k}^2 - C_1^2) (B_{2k}^2 - C_2^2) - 2 (B_{1k} B_{2k} + C_1 C_2) \Delta^2 + \Delta^4 \right] = 0, \]

we obtain the two Bogoliubov spectra,
\[ E_{\pm}^2 (k) = \left[ A_+ (k) - \Delta^2 \right] \pm \sqrt{A_-^2 (k) + \Delta^2 \left[ (C_1 + C_2)^2 - (B_{1k} - B_{2k})^2 \right]}, \quad (17) \]

and hence
\[ (B_{1k=0} - C_1) (B_{2k=0} - C_2) = \Delta^2. \quad (23) \]

As the last term in Eq. (16) can be rewritten as the product of \( (B_{1k} - C_1) (B_{2k} - C_2) - \Delta^2 \) and \( (B_{1k} + C_1) (B_{2k} + C_2) - \Delta^2 \), the term is zero at zero momentum \( k = 0 \). Thus, we confirm that at least one of the two Bogoliubov spectra is gapless. This is anticipated from the \( U(1) \) symmetry breaking of the system. On the other hand, it is straightforward to rewrite the condensate thermodynamic potential in the form,
\[ \Omega_0 = -\frac{\Delta^2}{g_{12}} - \frac{C_1^2}{2g_{11}} - \frac{C_2^2}{2g_{22}}. \quad (24) \]

We now turn to consider the action for quantum fluctuations \( S_B \), which gives the LHY contribution to the
thermodynamic potential \[\Omega\],

\[
\Omega_{\text{LHY}} = \frac{k_B T}{2} \sum_{\mathbf{q}, i\omega_n} \ln \det \left[ -\mathcal{D}^{-1}(\mathbf{q}, i\omega_n) \right] e^{i\omega_n 0^+}, \tag{25}
\]

\[
= \frac{1}{2} \sum_{\mathbf{k}} \left[ E_\mathbf{k}^+ + E_\mathbf{k}^- - B_{1\mathbf{k}} - B_{2\mathbf{k}} \right]. \tag{26}
\]

In two and three dimensions, it is worth noting that both \(\Omega\) and \(\Omega_{\text{LHY}}\) have ultraviolet divergence. However, these two divergences can cancel with each other exactly, once the regularization of the bare interaction strengths \(g_{ij}\) is applied. This will be discussed in more details when we explicitly write down the total thermodynamic potential in different dimensions.

### B. Equal intra-species interactions

For simplicity, from now on, let us concentrate on the case with equal intra-species interactions \(g_{11} = g_{22} = g\). With symmetric intra-species interactions, it is natural to take the same population for bosons in different species, i.e., \(\phi_{1c} = \phi_{2c}\). Therefore, we have \(C_1 = C_2 = C = \mu + \Delta > 0\) and \(B_{1\mathbf{k}} = B_{2\mathbf{k}} = B_{\mathbf{k}} = \varepsilon_{\mathbf{k}} + C + \Delta\). It is easy to find the two Bogoliubov spectra,

\[
E_\mathbf{k}^- = \sqrt{\varepsilon_{\mathbf{k}} (\varepsilon_{\mathbf{k}} + 2C + 2\Delta)}, \tag{27}
\]

\[
E_\mathbf{k}^+ = \sqrt{\varepsilon_{\mathbf{k}} + 2C} (\varepsilon_{\mathbf{k}} + 2\Delta). \tag{28}
\]

The upper Bogoliubov branch \(E_\mathbf{k}^+(\mathbf{k})\) is thereby gapped, provided the pairing gap \(\Delta \neq 0\). Finally, the total thermodynamic potential takes the form,

\[
\Omega = -\frac{C^2}{g} \frac{\Delta^2}{g_{12}} + \frac{1}{2} \sum_{\mathbf{k}} \left[ E_\mathbf{k}^+ + E_\mathbf{k}^- - 2B_{\mathbf{k}} \right]. \tag{29}
\]

For a given chemical potential \(\mu\), the saddle-point value of the pairing gap \(\Delta_0\) is to be determined by minimizing the thermodynamic potential, i.e.,

\[
\left. \frac{\partial \Omega}{\partial \Delta} \right|_{\Delta_0} = 0. \tag{30}
\]

We then calculate the total number of bosons in the droplet using the number equation,

\[
n = -\frac{\partial \Omega (\mu, \Delta_0)}{\partial \mu}, \tag{31}
\]

and obtain the total energy of the droplet \(E = \Omega + n\mu\).

### III. BOGOLIUBOV THEORY AND PETROV’S PRESCRIPTION

It is useful to explicitly compare the structure of our pairing theory with that of the widely-used Petrov theory. For this purpose, here we briefly review the Petrov’s prototype theory of quantum droplets. Within the Bogoliubov approximation \([\text{35}]\), we decouple the inter-species interaction Hamiltonian density \((\phi_{1c} = \phi_{2c} = \phi_c)\),

\[
g_{12} \phi_1 \phi_2 \phi_1 \phi_2 \simeq \frac{D_2^2}{g_{12}} - D (\delta \phi_1 \delta \phi_1 + \delta \phi_2 \delta \phi_2) - D (\delta \phi_1 \delta \phi_2 + \delta \phi_1 \delta \phi_2 + H.c.), \tag{32}
\]

where H.c. stands for taking the Hermitian conjugate and \(D = -g_{12} \phi_c^2 \) > 0 seems to play the role of the pairing field \(\Delta\) in our pairing theory. However, there is a slight difference. The Bogoliubov decoupling shown in the above generates two additional terms in the quantum fluctuation action \(S_B\), i.e., \(-\int dx D (\delta \phi_1 \delta \phi_1 + \delta \phi_2 \delta \phi_2)\) and \(-\int dx D (\delta \phi_1 \delta \phi_2 + \delta \phi_2 \delta \phi_1)\). In momentum space, the inverse Green function of bosons \(\mathcal{D}^{-1}(\mathbf{k}, \omega)\) then becomes,

\[
\mathcal{D}^{-1} = \begin{bmatrix}
\omega - B_{\mathbf{k}} & -C & D & D \\
-C & -\omega - B_{\mathbf{k}} & D & D \\
D & D & \omega - B_{\mathbf{k}} & -C \\
D & D & -C & -\omega - B_{\mathbf{k}}
\end{bmatrix}, \tag{33}
\]

where \(B_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu + 2C - D\). The existence of the two additional terms leads to the two Bogoliubov spectra,

\[
\mathcal{E}_\mathbf{k}^\pm = \sqrt{(B_{\mathbf{k}} - C)(B_{\mathbf{k}} + C + 2D)}. \tag{34}
\]

Here, we have used the tilde to distinguish the dispersion relations from those of the pairing theory. In this case, it is easy to see that the condensate thermodynamic potential takes the form,

\[
\Omega_0 = -2\mu \phi_c^2 + g_1 \phi_1^2 + g_2 \phi_2^2. \tag{35}
\]

By minimizing \(\Omega_0\) with respect to \(\phi_c^2\), we obtain the restriction,

\[
\mu = g_1 \phi_1^2 + g_2 \phi_2^2 = C - D, \tag{36}
\]

or equivalently \(B_{\mathbf{k}=0} = C\), which ensures the gapless Bogoliubov spectra. Therefore, we may rewrite down the condensate thermodynamic potential,

\[
\Omega_0 = \frac{C^2}{g} - \frac{D^2}{g_{12}}, \tag{37}
\]

the two dispersion relations,

\[
\mathcal{E}_\mathbf{k}^- = \sqrt{\varepsilon_{\mathbf{k}} (\varepsilon_{\mathbf{k}} + 2C + 2D)}, \tag{38}
\]

\[
\mathcal{E}_\mathbf{k}^+ = \sqrt{\varepsilon_{\mathbf{k}} (\varepsilon_{\mathbf{k}} + 2C - 2D)}, \tag{39}
\]

and also the LHY thermodynamic potential,

\[
\Omega_{LHY} = \frac{1}{2} \sum_{\mathbf{k}} \left[ \mathcal{E}_\mathbf{k}^+ + \mathcal{E}_\mathbf{k}^- - 2 (\varepsilon_{\mathbf{k}} + C) \right]. \tag{40}
\]

In three dimensions, using Eq. \([\text{4}]\) we replace the bare interaction strengths \(g\) and \(g_{12}\) with the s-wave scattering
lengths \( a \) and \( a_{12} \), respectively. Therefore, we obtain \( \Omega_{3D} = \Omega_0 + \Omega_{LHY} \),
\[
\Omega_{3D} = -\frac{m}{4\pi \hbar^2} \left[ \frac{C^2}{a} + \frac{D^2}{a_{12}} \right] + \frac{1}{2} \sum_{\mathbf{k}} \left[ \tilde{E}_+ (\mathbf{k}) + \tilde{E}_- (\mathbf{k}) \right] - 2(\varepsilon_k + C) + \frac{2(C^2 + D^2)}{\hbar^2 k^2/m}.
\]
(41)
The integration over the momentum can be easily calculated, by using the identity
\[
\sum_{\mathbf{k}} \left[ \sqrt{\varepsilon_k(\varepsilon_k + \alpha) - \varepsilon_k - \frac{\alpha^2}{2\varepsilon_k}} \right] = \left( \frac{2m}{\alpha} \right)^{3/2} \frac{\alpha^{5/2}}{15\pi^2 \hbar^3}
\]
in three dimensions. We arrive at,
\[
\Omega_{3D} = -\frac{m}{4\pi \hbar^2} \left[ \frac{C^2}{a} + \frac{D^2}{a_{12}} \right] + \frac{8m^{3/2}C^{5/2}}{15\pi^2 \hbar^3} F_3 \left( \frac{D}{C} \right),
\]
(42)
where \( F_3(\alpha) \equiv (1 + \alpha)^{5/2} + (1 - \alpha)^{5/2} \). To calculate the total energy, we note that unlike the pairing gap \( \Delta \)
in our pairing theory, the variable \( C \) is not a variational parameter. Therefore, there is an ambiguity to determine the variables \( D \) and then \( C = \mu + D \) for a given chemical potential \( \mu \). Nevertheless, we may assume that
\[
\frac{D}{C} = \frac{g_{12}}{\mu} \approx -\frac{a_{12}}{a},
\]
(44)
so that \( C = \mu a/(a + a_{12}) \) and \( D = -\mu a_{12}/(a + a_{12}) \). As quantum droplets emerge when \( D/C = -a_{12}/a > 1 \) in three dimensions, we immediately find that the Bogoliubov spectrum \( E_+(\mathbf{k}) = \sqrt{\varepsilon_k(\varepsilon_k + 2C - 2D)} \) becomes complex and consequently the function \( F_3(\alpha) \) in Eq. (43) is ill-defined. To cure this problem, we may simply set \( \alpha = D/C = 1 \) in the function \( F_3(\alpha) \) and hence the LHY term become independent on the inter-species interaction strength. This Petrov’s prescription is now widely taken in the theoretical studies of quantum droplets. We note also that, to calculate the total energy, we may further approximate \( C = (2\pi \hbar^2 a/m)n \) and \( \mu = (2\pi \hbar^2 (a + a_{12})/m)n \), which leads to the total energy,
\[
\frac{E_{3D}}{N} = \frac{\pi \hbar^2 (a + a_{12})}{m}n + \frac{256\sqrt{\pi} \hbar^2 a^{5/2}}{15} m^{-1/2} n^{3/2}.
\]
(45)
In other words, to determine the density \( n \), we take the derivative of the first term in Eq. (43) only with respect to the chemical potential \( \mu \). This approximation is well justified for a conventional weakly-interacting Bose gas in three dimensions. However, it may not be convincing for quantum droplets, where the second term in Eq. (43) may become comparable to the first term.

**IV. THREE-DIMENSIONAL QUANTUM DROPLETS**

Let us now discuss the results of our pairing theory in three dimensions and show some technical details behind our previous work. By regularizing the bare interaction strengths \( g \) and \( g_{12} \) in terms of the \( s \)-wave scattering lengths \( a \) and \( a_{12} \), we rewrite the thermodynamic potential Eq. (20) into the form,
\[
\Omega_{3D} = -\frac{m}{4\pi \hbar^2} \left[ \frac{C^2}{a} + \frac{\Delta^2}{a_{12}} \right] + \frac{1}{2} (\mathcal{I}_+ + \mathcal{I}_-),
\]
(46)
\[
\mathcal{I}_+ = \sum_{\mathbf{k}} \left[ E_+ (\mathbf{k}) - (\varepsilon_k + C + \Delta) + \frac{C^2 + \Delta^2}{2\varepsilon_k} \right]
\]
(47)
\[\mathcal{I}_- \]
can be directly calculated, with the help of the identity Eq. (12),
\[
\mathcal{I}_- = \frac{16m^{3/2}}{15\pi^2 \hbar^3} C^{5/2} \left( 1 + \frac{\Delta}{C} \right)^{5/2}.
\]
(48)
To calculate \( \mathcal{I}_+ \), we introduce a new variable \( t = [\hbar^2 k^2/(2m)]/(2C) \) and \( \alpha \equiv \Delta/C \) and rewrite
\[
\mathcal{I}_+ = \frac{16m^{3/2}}{15\pi^2 \hbar^3} C^{5/2} h_3 (\alpha),
\]
(49)
where the function
\[
\frac{h_3 (\alpha)}{\Delta} \equiv \frac{15}{4} \int_0^\infty dt \sqrt{t} \left[ \sqrt{(t + 1)(t + \alpha) - t} - \frac{1 + \alpha}{2} + \frac{(1 - \alpha)^2}{8t} \right].
\]
(50)
By combining \( \mathcal{I}_+ \) and \( \mathcal{I}_- \), we obtain the (regularized) LHY thermodynamic potential \( (C = \mu + \Delta) \),
\[
\Omega_{LHY} = \frac{8m^{3/2}}{15\pi^2 \hbar^3} (\mu + \Delta)^{5/2} g_{12} \left( \frac{\Delta}{\mu + \Delta} \right),
\]
(51)
\[ \alpha > \text{is not well-defined for} \]

where \( G_3(\alpha) \equiv (1 + \alpha)^{5/2} + h_3(\alpha) \). Compared with the function \( F_3(\alpha) \equiv (1 + \alpha)^{5/2} + (1 - \alpha)^{5/2} \) in the last section, we find interestingly that the role of \((1 - \alpha)^{5/2}\), which is not well-defined for \( \alpha > 1 \), is now taken by the new function \( h_3(\alpha) \). In Fig. 4 we show the function \( h_3(\alpha) \). It is slightly larger than \((1 - \alpha)^{5/2}\) in the interval \( \alpha \subseteq [0, 1] \). Therefore, we obtain the total thermodynamic potential,

\[
\Omega_{3D} = -\frac{m}{4\pi \hbar^2} \left[ \frac{(\mu + \Delta)^2}{a} + \frac{\Delta^2}{a_{12}} \right] + \frac{8n_{s}^{3/2}}{15\pi^2 \hbar^2} \left( \mu + \Delta \right)^{5/2} G_3 \left( \frac{\Delta}{\mu + \Delta} \right). \tag{52}
\]

It takes essentially the same form as the thermodynamic potential Eq. (43) in the standard Bogoliubov theory, except that the ill-defined function \( F_3(\alpha) \) is now replaced by \( G_3(\alpha) \), and the pairing gap \( \Delta \) is variational and should be determined by minimizing \( \Omega_{3D}(\Delta) \).

For a given chemical potential \( \mu \), we therefore minimize \( \Omega_{3D} \) to find the saddle-point value of the pairing order parameter \( \Delta_0 \). In Fig. 2 we show the thermodynamic potential \( \Omega_{3D} \) as a function of \( \Delta \) at the inter-species interaction strength \( a_{12} = -1.10a \). The curves at three different chemical potentials \( \mu = 0, -0.06, \text{and} -0.08 \), measured in units of \( 10^{-10}h^2/(2ma^2) \), are plotted. When the chemical potential is above a critical value, i.e., \( \mu_c \simeq -8.0 \times 10^{-6}h^2/(2ma^2) \), we typically find a global minimum in the thermodynamic potential at \( \Delta_0 \neq 0 \). For \( \mu < \mu_c \), the global minimum turns into a local minimum and hence the saddle-point pairing parameter takes the trivial solution \( \Delta_0 = 0 \). As a result, there is a jump in

\[ \Delta_0 \text{when we tune the chemical potential across} \mu_c. \]

Physically, this indicates a first-order quantum phase transition from a droplet phase to a collapsing phase. In other words, when the density \( n \) is very dilute (at \( \mu < \mu_c \)), the repulsive force provided by quantum fluctuations (i.e., the LHY energy \( \propto n^{3/2} \)) is unstable to balance the attractive mean-field force (i.e., characterized by the mean-field energy \( \propto n^2 \)). Thus, the mean-field collapse can no longer be prevented. The critical density \( n_c \) at the chemical potential \( \mu_c \) corresponds to the spinodal point where the spinodal instability sets in.

For nonzero \( \Delta_0 \neq 0 \), we obtain \( \Omega_{3D}(\mu, \Delta_0) \) and calculate \( n = -\partial \Omega_{3D}(\mu, \Delta_0)/\partial \mu \). In Fig. 3 we show the chemical potential \( \mu > \mu_c \), the parameter \( C = \mu + \Delta_0 \) and the pairing gap \( \Delta_0 \) as a function of the density \( n > n_c \), at the inter-species interaction strength \( a_{12} = -1.10a \). The positive slope of the density equation of state \( \mu(n) \), i.e., \( \partial n/\partial \mu > 0 \), indicates that the compressibility of the droplet is positive and the system is indeed mechanically stable, as we anticipate. Remarkably, at small densities we find numerically that the chemical potential is much smaller than either the parameter \( C \) or the pairing gap \( \Delta_0 \). This could be easily understood from the \( \Delta \)-dependence of \( \Omega_0 \) and \( \Omega_{LHY} \), as shown in Eq. (52). We note that two terms in \( \Omega_0 \) are large and have opposite sign. Each of them (i.e., absolute value) is much larger than \( \Omega_{LHY} \). Therefore, when we minimize \( \Omega \) with respect to \( \Delta \), we only need to minimize \( \Omega_0 \). This leads to the condition,

\[
\mu + \frac{\Delta_0}{a} + \frac{\Delta_0}{a_{12}} \simeq 0. \tag{53}
\]

Hence, as a result of \( a_{12} \sim -a \), we obtain

\[
\mu \simeq - \left( 1 + \frac{a}{a_{12}} \right) \Delta_0 \ll \Delta_0, C. \tag{54}
\]
Therefore, we obtain, the energy for small densities, proximate the energy functional obtained by Petrov using his prescription of the density at the interspecies interaction strengths $\mu$ calculate $E$ and also the term $\Delta - \Delta^0$ dependence in the field energy becomes different from the widely-accepted conventional expression. As the beyond-mean-field LHY effect becomes dominant in quantum droplets, a consistent treatment of the potential regularization is necessary. Therefore, it is not a surprise why our regularized mean-field energy becomes different from the widely-accepted conventional expression.

In Fig. 4 we report the energy per particle as a function of the density at two inter-species interaction strengths $a_{12} = -1.05a$ (a) and $a_{12} = -1.50a$ (b). Our pairing results (numerical - thick brown solid lines and analytical - black thin solid lines) are compared with the recent DMC data (circles) [28] and the MF+LHY predictions with Petrov’s prescription Eq. (40) (dashed lines). We note that the units of energy and density change a lot in the upper and lower panels.

Due to the smallness of $|\mu|$, it is reasonable to neglect the $\mu$-dependence in $\Omega_{3D}^{LHY}$ and also the term $\mu^2$ in $\Omega_0$. Therefore, we obtain,

$$\Omega_{3D} \simeq - \frac{m}{4\pi \hbar^2} \left[ \frac{2\mu \Delta + \Delta^2}{a} + \frac{\Delta^2}{a_{12}} \right] + \frac{32\sqrt{2}m^{3/2}}{15\pi^2 \hbar^3} \Delta^{5/2}. \tag{55}$$

By taking the derivative with respect to $\mu$ and taking the saddle-point value $\Delta = \Delta_0$, we find

$$n = - \frac{\partial \Omega_{3D}}{\partial \mu} \simeq \frac{m}{2\pi \hbar^2 a} \Delta_0. \tag{56}$$

Replacing $\Delta_0$ by the density $n$ everywhere in $\Omega_{3D}$ and calculate $E_{3D} = \Omega_{3D} + \mu n$, we finally arrive at an approximate energy for small densities,

$$\frac{E_{3D}}{N} = - \frac{\pi \hbar^2}{m} \left( a + \frac{a^2}{a_{12}} \right) n + \frac{32\sqrt{2}\pi \hbar^2 a^{5/2}}{15m} n^{3/2}. \tag{57}$$

It is useful to compare this analytic expression with the energy functional obtained by Petrov using his prescription [3], i.e., Eq. (15) It is interesting to see that these two energy functionals have the exactly same LHY term. The reproduce of the Petrov’s approximate LHY term in our pairing theory suggests that Petrov’s prescription is actually very reasonable, at least for the case of equal intra-species interactions considered here [33]. However, it is worth emphasizing that, quite unexpectedly, the mean-field energy term in our pairing theory (i.e., the first term in Eq. (57)) changes a lot. It is weakened by a factor of $-a/a_{12} < 1$, compared with the conventional mean-field expression

$$\frac{(g + g_{12}) n}{m} \rightarrow \frac{\pi \hbar^2 (a + a_{12})}{m} n. \tag{58}$$

This difference partly comes from our regularization of the bare interaction strengths, which is rigorously treated in the pairing theory. As the beyond-mean-field LHY effect becomes dominant in quantum droplets, a consistent treatment of the potential regularization is necessary. Therefore, it is not a surprise why our regularized mean-field energy becomes different from the widely-accepted conventional expression.

In Fig. 4 we report the energy per particle as a function of the density at two inter-species interaction strengths: $a_{12} = -1.05a$ (a) and $a_{12} = -1.50a$ (b). Our pairing results (numerical - thick brown solid lines and analytical - black thin solid lines) are compared with the latest DMC data (circles) and the Petrov’s energy functional Eq. (15) (red dashed lines). At small densities close to the equilibrium density, where the energy per particle takes minimum (or the pressure is zero), we find an excellent agreement between our analytical result and the full numerical result, confirming the usefulness of the analytic energy functional Eq. (57). Both results agree reasonably well the benchmark DMC data. As our pairing theory is variational and thus provides an upper bound for the energy, it is impressive to see such a good agreement, particularly for small inter-species attractions, as shown in (4a). In contrast, Petrov’s energy functional Eq. (15) predicts smaller energy than the DMC simulations. With increasing inter-species attractions, the under-estimation in Petrov’s energy becomes very significant as seen from (4b). We note that, there is also a notable difference between our pairing result and the DMC data at large attractive inter-species attractions, since the density becomes large (i.e., $na^3 \sim 0.001$) and the effect beyond LHY-correction [14] should be taken into account.

V. ONE-DIMENSIONAL QUANTUM DROPLETS

We now turn to consider low-dimensional quantum droplets, starting from the one-dimensional case. In one dimension, the contact interaction is well defined and does not need regularization. The interaction strength can be characterized by using the dimensionless interaction parameter, such as $\gamma = mg/(\hbar^2) = -2/(na)$ and

![Graph](https://via.placeholder.com/150)

**FIG. 4.** Three-dimensional energy per particle as a function of the density at the interspecies interaction strengths $a_{12} = -1.05a$ (a) and $a_{12} = -1.50a$ (b). Our pairing results (numerical - thick brown solid lines and analytical - black thin solid lines) are compared with the recent DMC data (circles) and the MF+LHY predictions with Petrov’s prescription Eq. (40) (dashed lines). We note that the units of energy and density change a lot in the upper and lower panels.
The function $h_1(\alpha)$ (solid line) and its comparison to $(1 - \alpha)^{3/2}$ (dashed line).

\begin{equation}
\eta = mg_{12}/(nh^2) = -2/(na_{12}), \text{ where}
\end{equation}

\begin{align}
a &= -\frac{2\hbar^2}{mg} < 0 \\
a_{12} &= -\frac{2\hbar^2}{mg_{12}} > 0
\end{align}

are the one-dimensional s-wave scattering lengths. Following Ref. [27], we choose the binding energy of a dimer as before in two bosons in different species, i.e.,

\begin{equation}
\varepsilon_B = \frac{\hbar^2}{ma_{12}},
\end{equation}

as the units of energy, and the inverse scattering length $|a|^{-1}$ as the units of density.

In the Bogoliubov theory, the LHY thermodynamic potential Eq. (40) in one dimension is easy to calculate. By performing the one-dimensional integration,

\begin{equation}
\sum_k \left[ \sqrt{\varepsilon_k (\varepsilon_k + \alpha)} - \varepsilon_k - \frac{\alpha}{2} \right] = -\frac{(2m)^{1/2} \alpha^{3/2}}{3\pi \hbar},
\end{equation}

we obtain

\begin{equation}
\Omega_{LHY} = -\frac{2m^{1/2}}{3\pi \hbar} \left[ (C + D)^{3/2} + (C - D)^{3/2} \right].
\end{equation}

By taking $C = gn/2$ and $D = g_{12}n/2$ as before in $\Omega_{LHY}$ and adding the mean-field energy $(g + g_{12})n^2/4$, we obtain the energy per particle predicted by the Bogoliubov theory,

\begin{equation}
\frac{E_{1D}}{N} = (g + g_{12}) \frac{n}{4} - \frac{(2m)^{1/2}}{6\pi \hbar} g^{3/2} F_1 \left( \frac{g_{12}}{g} \right) n^{1/2},
\end{equation}

where $F_1(\alpha) \equiv (1 + \alpha)^{3/2} + (1 - \alpha)^{3/2}$. It is interesting to note that, in one dimension the LHY energy functional is negative so the force provided by quantum fluctuations is attractive. It is to be balanced by the repulsive mean-field force at $g > -g_{12} > 0$. Therefore, somehow counterintuively, the formation of quantum droplets is driven by quantum fluctuations [18]. As the mean-field solution is stable, the energy in Eq. (64) does not suffer from the issue of complex number as we encounter earlier in three dimensions. Nevertheless, following Ref. [18] we may still use the Petrov’s prescription and take $g_{12} = -g$ in Eq. (64) to define an energy per particle,

\begin{equation}
\frac{E_{1D}}{N} = (g + g_{12}) \frac{n}{4} - \frac{2m^{1/2}}{3\pi \hbar} g^{3/2} n^{1/2}.
\end{equation}

In the pairing theory, we calculate the thermodynamic potential Eq. (29) in one dimension. As in the three-dimensional case, we similarly separate the LHY thermodynamic potential into two parts, $\mathcal{I}_-$ and $\mathcal{I}_+$. It is straightforward to obtain $\mathcal{I}_-$ with the help of the identity Eq. (52) and we obtain,

\begin{equation}
\mathcal{I}_- = -\frac{4m^{1/2}}{3\pi \hbar} C^{3/2} \left( 1 + \frac{\Delta}{C} \right)^{3/2}.
\end{equation}

For $\mathcal{I}_+$, we instead find

\begin{equation}
\mathcal{I}_+ = \frac{4m^{1/2}}{3\pi \hbar} C^{3/2} h_1(\alpha),
\end{equation}

where the function $h_1(\alpha)$ is given by,

\begin{equation}
h_1 \equiv 3 \int_0^\infty dt \left[ t^2 + \frac{1 + \alpha}{2} - \sqrt{(t^2 + 1)(t^2 + \alpha)} \right].
\end{equation}
and is plotted in Fig. 7. Therefore, we obtain the total thermodynamic potential \( \Omega_{1D} = -\frac{C^2}{g} - \frac{\Delta^2}{g_{12}} - \frac{4m^{1/2}}{3\pi \hbar} C^{3/2} G_1 \left( \frac{\Delta}{C} \right) \), (69)

where \( G_1(\alpha) \equiv (1 + \alpha)^{3/2} + h_1(\alpha) \). As shown in Fig. 7, the thermodynamic potential in one dimension typically exhibits a global minimum as a function of the pairing gap \( \Delta \), similar to the three-dimensional case.

By finding the saddle-point solution \( \Delta = \Delta_0 \neq 0 \) through the minimization of \( \Omega(\Delta) \), we consequently calculate the density \( n = -\partial \Omega(\mu, \Delta_0)/\partial \mu \). The resulting parameter \( C = \mu + \Delta_0 \) and the pairing gap \( \Delta_0 \), together with the chemical potential \( \mu \), are shown in Fig. 7 as a function of the density \( n \), at a typical inter-species interaction strength \( g_{12} = -0.75g \). Here, we are always in the weak-coupling regime, since the dimensionless interaction parameters such as \( \gamma = 2/(n|a|) < 1 \). Unlike the three-dimensional case, the condition \( |\mu| \ll C, \Delta_0 \) seems to be less satisfied at low densities, where we can see a clear difference between \( C \) and \( \Delta_0 \). Therefore, although an approximate analytical energy equation can still be derived, i.e.,

\[
\frac{E_{1D}}{N} = -\left( g + \frac{g^2}{g_{12}} \right) \frac{n}{4} - \frac{2m^{1/2}}{3\pi \hbar} g^{3/2} n^{1/2},
\]

we would prefer to use the full numerical calculation. A comparison between the numerical and analytical results of our pairing theory at the inter-species interaction strength \( g_{12} = -0.75g \) is shown in Appendix A.

In Fig. 8 we present the energy per particle predicted by the pairing theory at three interspecies interactions \( g_{12}/g = -0.60 \) (black), \( -0.75 \) (red) and \( -0.90 \) (blue) by solid lines, and compare them to the available DMC data taken from Ref. 27 (symbols), to the Bogoliubov results Eq. 64 (dashed lines), and to the MF+LHY results with Petrov’s prescription Eq. 65 (dashed line, for \( g_{12}/g = -0.75 \) only). The energy is in units of \( \epsilon_B/2 \) and the density is in units of \( |a|^{-1} \).

FIG. 7. One-dimensional chemical potential \( \mu \), the parameter \( C \) and the pairing gap \( \Delta_0 \), in units of \( \epsilon_B \), as a function of the total density \( n \) (in units of \( |a|^{-1} \)) at \( g_{12} = -0.75g \).

FIG. 8. One-dimensional energy per particle as a function of the density at three interspecies interaction strengths \( g_{12}/g = -0.60 \) (black), \( -0.75 \) (red) and \( -0.90 \) (blue). Our pairing results (solid lines) are compared with the recent DMC data (symbols) 27, the MF+LHY predictions Eq. 64 (dotted-dashed lines), and the MF+LHY results with Petrov’s prescription Eq. 65 (dashed line, for \( g_{12}/g = -0.75 \) only). The energy is in units of \( \epsilon_B/2 \) and the density is in units of \( |a|^{-1} \).

FIG. 9. Minimum energy per particle \( E_{\text{min}}/N \) or equilibrium chemical potential \( \mu_{\text{eq}} \) in one dimension as a function of the interspecies interaction strength \( g_{12}/g \), obtained from the pairing theory (solid line), the DMC simulation (circles) 27 and the MF+LHY theory Eq. 65 (dot-dashed line). The energy is in units of \( \epsilon_B/2 \).
close to unity so the dimensionless interaction parameter \( \gamma = 2/(n |a|) \sim O(1) \) is large. We would rather anticipate the breakdown of the Bogoliubov approximation, which our pairing theory relies on. Indeed, at this interaction strength the conventional Bogoliubov prediction Eq. (64) already shows significant deviation from the DMC data. We attribute the good agreement between our theory and the DMC simulation to our reasonable description of the bosonic pairing.

To understand this, it is useful to show the chemical potential \( \mu_{\text{eq}} \) at the equilibrium density (or the minimum energy per particle \( E_{\text{min}}/N \)) as a function of the inter-species interaction strength \( g_{12}/g \), as reported in Fig. 3. The excellent agreement between our pairing theory and the DMC prediction [27] and the few-body zero-crossing of dimer-dimer scattering, we find the equilibrium density vanishes at \( g_{12}/g \) near the zero-crossing of dimer-dimer interaction \( (g_{12}/g)_{\text{crit}} \sim -0.47(2) \) as predicted by the DMC [27]. Towards the critical interaction strength, the equilibrium chemical potential quickly approaches the half of the binding energy of a dimer, i.e., \( \mu_{\text{eq}} \sim -\varepsilon_B/2 \), indicating that the system could be understood as a collection of weakly-interacting dimers. This interpretation is reasonable, as the DMC threshold \((g_{12}/g)_{\text{threshold}} \sim (g_{12}/g)_{\text{crit}} \sim -0.47(2)\) is close to the zero-crossing in the effective dimer-dimer interaction \((g_{12}/g)_{\text{crit}} \sim -0.35\), which seems to be consistent with the DMC prediction [27] and the few-body zero-crossing result [32].

Our pairing theory precisely provides a useful description of those weakly-interacting dimers at the mean-field level, since we take a uniform pairing gap in the species interactions near the zero-crossing of dimer-dimer scattering. By determining the equilibrium density \( n_{\text{eq}} \) at different inter-species interactions near the zero-crossing of dimer-dimer scattering, we find the equilibrium density vanishes at \((g_{12}/g)_{\text{crit}} \sim -0.35\), which seems to be consistent with the DMC prediction [27] and the few-body zero-crossing result [32].

**VI. TWO-DIMENSIONAL QUANTUM DROPLETS**

We finally consider two-dimensional quantum droplets. In two dimensions, the regularization of the bare interaction strength becomes subtle due to the logarithmic infrared divergence at low energy, which we may remove by introducing an arbitrary energy scale \( \varepsilon_c \), i.e.,

\[
\frac{1}{g} = \frac{m}{4\pi \hbar^2} \ln \left( \frac{4\hbar^2}{e^{2\gamma} m a^2 \varepsilon_c} \right) - \sum_k \frac{1}{2\varepsilon_k + \varepsilon_c},
\]

\[
\frac{1}{g_{12}} = \frac{m}{4\pi \hbar^2} \ln \left( \frac{4\hbar^2}{e^{2\gamma} m a^2_{12} \varepsilon_c} \right) - \sum_k \frac{1}{2\varepsilon_k + \varepsilon_c}.
\]

Here, \( \gamma \approx 0.577216 \) is Euler–Mascheroni constant, \( a \) and \( a_{12} \) are two-dimensional \( s \)-wave scattering lengths. Alternatively, we may consider the use of the binding energies \( E_T = 4\hbar^2/(e^{2\gamma} m a^2) \) and \( E_S = 4\hbar^2/(e^{2\gamma} m a_{12}^2) \),

**FIG. 10.** Two-dimensional thermodynamic potential \( \Omega_{2D} \), in units of \( 10^{-6}E_T a^{-2} \), as a function of the pairing parameter \( \Delta \), at different chemical potentials \( \mu = 1.0 \) (solid line), 0 (dashed line), and \(-0.2 \) (dot-dashed line), and at the inter-species interaction strength \( \ln(a_{12}/a) \approx 5 \). Both \( \Delta \) and \( \mu \) are measured in units of \( 10^{-3}E_T \).

where analogous to the fermionic case the subscripts “\( T \)” and “\( S \)” emphasize the tendency of the formation of triplet and singlet pairs for bosons in the same-species and unlike-species, respectively. We then rewrite the bare interaction strengths in a simpler form,

\[
\frac{1}{g} = -\sum_k \frac{1}{\hbar^2 k^2/m + E_T},
\]

\[
\frac{1}{g_{12}} = -\sum_k \frac{1}{\hbar^2 k^2/m + E_S}.
\]

In this section, we use \( E_T \) and \( a^{-2} \) as the units of energy and density, respectively.

In the Bogoliubov theory, the approximate energy of quantum droplets was derived by Petrov and Astrakharchik in Ref. [18]. For \( \ln(a_{12}/a) \gg 1 \), it takes the form [18],

\[
\frac{E_{2D}}{N} = \frac{2\pi n}{\ln^2 (a_{12}/a)} \left[ \ln \left( \frac{n}{n_{\text{eq}}} \right) - 1 \right],
\]

where the equilibrium density is

\[
n_{\text{eq}} a^2 = e^{-2\gamma-3/2} \ln(a_{12}/a)/(a_{12}/a).
\]

In our pairing theory, by replacing the bare interaction strengths with the binding energies, the thermodynamic potential can be written as \( (C = \mu + \Delta) \),

\[
\Omega_{2D} = \frac{1}{2} \sum_k \left[ E_+ (k) + E_- (k) - 2 (\varepsilon_k + C + \Delta) \right.
\]

\[
+ \frac{2C^2}{2\varepsilon_k + E_T} + \frac{2\Delta^2}{2\varepsilon_k + E_S} \right],
\]
The same trick was used in Ref. [18] to derive the Bogoliubov result Eq. (73). A vanishing condensate term is related to the fact that in two dimensions, the small interaction parameter is given by $1/\ln(na^2)$ and one has to include the LHY term in the energy, in order to have a meaningful perturbative expansion expression for the energy. As the controlling parameter is only logarithmically small, as we shall see, it appears more challenging to obtain an accurate result within perturbation theories.

The integration in Eq. (77) can be performed analytically, as in usual two-dimensional mean-field theories. We find that,

$$\Delta n_{2D} = \frac{m}{4\pi\hbar^2} \left[ C\Delta - C_2\sqrt{C\Delta} + \frac{\mu^2}{4} \ln \left( \sqrt{C + \sqrt{\Delta}} \right) \right. $$

$$\left. + \frac{C_2^2}{2} \ln (\epsilon C_2) - C^2 \ln E_T - \Delta^2 \ln E_S \right], \quad (78)$$

where $C_2 \equiv C + \Delta = \mu + 2\Delta$. In Fig. 10 we examine the $\Delta$-dependence of the thermodynamic potential at the inter-species interaction strength $\ln(a_{12}/a) = 5$. It clearly shows a global minimum when the chemical potential is above a threshold, similar to the three-dimensional and one-dimensional cases. Therefore, we determine the saddle-point pairing gap $\Delta_0$ and consequently calculate the density and total energy. The resulting parameter $C$ and the pairing gap $\Delta_0$ are shown in Fig. 11 as a function of the density $n$. The chemical potential $\mu$ is also shown. We find that with increasing the density, the chemical potential $\mu$ increases rapidly and is larger than the pairing gap $\Delta_0$ at sufficiently large densities.

In Fig. 12 we report the density dependence of the energy per particle of two-dimensional quantum droplets at two inter-species interaction strengths, $\ln(a_{12}/a) = 5$ (a) and $\ln(a_{12}/a) = 2$ (b). Our pairing results (solid lines) are compared with Petrov’s theory Eq. (75) (dashed line). In (a), we show also the DMC data from Ref. [18]. The energy is in units of the inter-species binding energy $E_S$ and the density is in units of $a^{-2}$. We note that the scales of energy and density change by a factor of $\sim 10$ in the upper and lower panels.

**FIG. 11.** Two-dimensional chemical potential $\mu$, the parameter $C$, and the pairing gap $\Delta_0$, in units of $10^{-3}E_T$, as a function of the total density $n$ (in units of $10^{-3}a^{-2}$) at $\ln(a_{12}/a) = 5$.

**FIG. 12.** Two-dimensional energy per particle as a function of the density at three interspecies interaction strengths $\ln(a_{12}/a) = 5$ (a), $\ln(a_{12}/a) = 2$ (b), and $\ln(a_{12}/a) = 1$ (inset in (b)). Our pairing results (solid lines) are compared with the MF+LHY predictions with Petrov’s theory Eq. (75) (dashed line). In (a), we show also the DMC data from Ref. [18]. The energy is in units of the inter-species binding energy $E_S$ and the density is in units of $a^{-2}$. We note that the scales of energy and density change by a factor of $\sim 10$ in the upper and lower panels.
In a Bose-Bose mixture, we determine a threshold in two dimensions, i.e., this threshold is close to the zero-crossing of the soliton-like many-particle bound state [47, 48]. Incidentally, this threshold is close to the zero-crossing \( \langle g_{12}/a \rangle_0 \sim 2.3 \) of the effective dimer-dimer interaction in two dimensions found through few-body calculations [39].

In future studies, it would be interesting to use our microscopic pairing theory to directly explore the profile and the collective excitations of quantum droplets, without the use of the local density approximation or density functional theories. These fundamental properties are important for characterizing ultradilute quantum droplets in ultracold atomic laboratories.

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Appendix A: Analytic energy expression in one dimension

In Fig. [12], we show the numerical and analytical results of our pairing theory for the one-dimensional energy per particle at the interspecies interaction strength \( g_{12} = -0.75 \). The analytical expression Eq. (70) does not provide a good approximation to the numerical result, since unlike in the three-dimensional case the assumption \( |\mu| \ll C_0 \) is not satisfied so well.
FIG. 13. One-dimensional energy per particle as a function of the density at the interspecies interaction strength $g_{12} = -0.75g$. Our pairing results (numerical - brown thick solid line, and analytical - black thin solid line, see Eq. (70)) are compared with the recent DMC data (symbols) [27], the MF+LHY prediction Eq. (64) (dot-dashed lines), and the MF+LHY results with Petrov’s prescription Eq. (65) (dashed line). The energy is in units of $\varepsilon_B/2$ and the density is in units of $|a|^{-1}$.

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