Self-bound quantum droplets: ground state and excitations

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This project aims to study the ground state properties and excitations of self-bound quantum droplets. The ground state is obtained by numerically solving the extended Gross-Pitaevskii equation, which takes into account quantum fluctuations. Then, using a Gaussian variational ansatz for the ground state, we calculate the values of the number of particles for which the droplet is metastable, obtaining results that agree with the numerical calculations. Furthermore, to study the excited states, we use the Bogoliubov-de Gennes approximation. This approximation assumes small oscillations of the wave function around the ground state. Once obtained the Bogoliubov equations, we solve them numerically to analyze the first excited state, the breathing mode. The results show that it is a bulk mode since the perturbation starts at the core of the droplet.

I. INTRODUCTION

At very low temperatures in the quantum regime, bosonic atoms (with integer spin) obey the Bose-Einstein statistics. When a gas of bosons is cooled down to temperatures close to 0K, a new state of matter arises: a Bose-Einstein condensate (BEC). It is characterized by a macroscopic occupation of the lowest single-particle state; atoms lose their individual identity and behave coherently as a single "superatom". The Bose-Einstein condensation is a quantum phenomenon that was predicted in 1924 by A. Einstein and S. N. Bose, but it wasn't observed for the first time until 1995. The first BEC was experimentally obtained by a research group at JILA using rubidium atoms confined in an external potential trap [1].

The reason why these experiments require low temperatures is the fact that, for a system to exhibit quantum behavior, there has to be an overlap of the wave functions of the atoms. In other words, the de Broglie wavelength has to be larger than the interatomic distance. To avoid recombination effects, the densities of these quantum systems are very low, therefore, the interatomic distances are large and the temperature must also be very low to obtain higher values of the de Broglie wavelength $\lambda_{dB} \propto 1/\sqrt{T}$.

Quantum droplets are small clusters of atoms that are self-bound by the balance of attractive and repulsive forces. In 2015, it was theoretically shown by Petrov [2] that the inclusion of quantum fluctuations could stabilize ultracold atomic gases from collapse, and that quantum droplets could be self-bound and exist without external confinement. A few years later, in 2018, the formation of quantum liquid droplets in a mixture of BECs was experimentally obtained [3].

The aim of this project is to study self-bound quantum droplets, their ground state properties, and their excited states through the Bogoliubov-de Gennes approximation.

II. SELF-BOUND QUANTUM DROPLETS

Quantum droplets are a self-bound state that stems from a BEC with attractive mean-field interactions that are balanced out by a repulsive beyond mean-field interaction. This beyond mean-field contribution originates from quantum fluctuations and stabilizes the system against the mean-field collapse, allowing it to exist without the presence of external trapping, i.e., self-bound [4]. The first exact calculation of the quantum fluctuations in bosonic atoms was carried out by T. Lee, K. Huang, and C. Yang in 1957, hence this term being referred to as the Lee-Huang-Yang (LHY) correction [5]. This beyond mean-field correction only depends on the two-body scattering length and this is why it is considered a universal term [2].

Moreover, in order to enable the delicate aforementioned balance, the mean-field interactions have to be of the same order of magnitude as the LHY term, and this is achieved by having competing interactions within the condensate. A one-component contact-interacting gas cannot be stabilized because the interacting force is too strong to be counterbalanced by quantum fluctuations. On the contrary, a two-component system can be stabilized since it has attractive and repulsive interaction forces that almost completely cancel out each other, and result in a small attractive mean-field force of the same order of magnitude as the LHY term [3].

These competing interactions can arise from a Bose-Bose contact-interacting mixture as mentioned before, but also from a dipolar quantum gas that exhibits both the contact interaction and the dipole-dipole interaction between the atoms [6]. In this study, we will focus on the case of Bose-Bose mixtures.

A. The extended Gross-Pitaevskii equation

Bose-Einstein condensates in the mean-field regime are described by means of the time-dependent Gross-

Pitaevskii equation (GPE):

$$i\hbar\partial_t\psi(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + g|\psi(\mathbf{r},t)|^2 + V_{\text{ext}}(\mathbf{r})\right]\psi(\mathbf{r},t)\,. \tag{1}$$

where $\psi(\mathbf{r},t)$ is the wave function of the BEC normalized to the total number of atoms N. The first and second terms of the equation are the kinetic energy and the interaction energy of the system, respectively, where $g = 4\pi\hbar^2 a_s/m$ with a_s the scattering length, and m the atomic mass. The third term is the external confining potential.

In a Bose-Bose mixture, the system is described by two coupled GPEs, one for each component. However, following Ref. [2], in the ground state and lowest-lying energy states, we can neglect the relative motion between the two components and consider a single-mode approximation, $\psi_i(\mathbf{r},t) = \sqrt{n_i^0}\,\phi(\mathbf{r},t)$, where n_i^0 is the equilibrium density of the ith component in the uniform case $(i = 1, 2)$.

After adding the dimensionless LHY correction $5/2\,|\phi|^3 - \tilde{\mu}$, setting the external trapping to zero $V_{\text{ext}} = 0$, and expressing the GPE in dimensionless form, it follows the extended GPE [2]:

$$i\partial_{\tilde{t}}\phi = (-\nabla^2_{\tilde{r}}/2 - 3|\phi|^2 + 5/2\,|\phi|^3 - \tilde{\mu})\phi\,, \tag{2}$$

where $\tilde{\mathbf{r}} = \mathbf{r}/\xi$, $\tilde{t} = t/\tau$, and $\tilde{\mu}$ is the dimensionless chemical potential. The length and time units, ξ and τ, are defined as follows:

$$\xi = \sqrt{\frac{3\sqrt{g_{22}}/m_1 + \sqrt{g_{11}}/m_2}{2|\delta g|\sqrt{g_{11}}\,n_1^0}}\,,\quad \tau = \frac{3\sqrt{g_{11}} + \sqrt{g_{22}}}{2|\delta g|\sqrt{g_{11}}\,n_1^0}. \tag{3}$$

The masses of the first and second components are defined by m_1 and m_2, respectively. The intra- and inter-species coupling constants are g_{11}, g_{22} and g_{12}; and $|\delta g|$ is defined as $|\delta g| = g_{12} + \sqrt{g_{11}g_{22}}$.

The ground state wave function, ϕ_0, is obtained by solving the time-independent extended GPE:

$$\left(-\nabla^2_{\tilde{r}}/2 - 3|\phi_0|^2 + 5/2\,|\phi_0|^3\right)\phi_0 = \tilde{\mu}\,\phi_0\,, \tag{4}$$

where $\tilde{\mu}$ can be obtained from the normalization condition $\tilde{N} = \int d\tilde{\mathbf{r}}\,|\phi_0|^2$. Moreover, $\tilde{N}$ can be written in terms of the number of particles of the i-component as $N_i = n_i^0\,\xi^3\tilde{N}$ [2].

We have numerically solved the time-independent extended GPE (4), by using the imaginary time step method [7], to obtain the ground state of a self-bound spherical droplet for different values of $\tilde{N}$.

In Fig. 1 we show the ground state wave function as a function of the radial coordinate. The stable droplets present a saturation density at the bulk region but only for values of $\tilde{N}$ higher than a threshold. This will be further investigated in the following section.

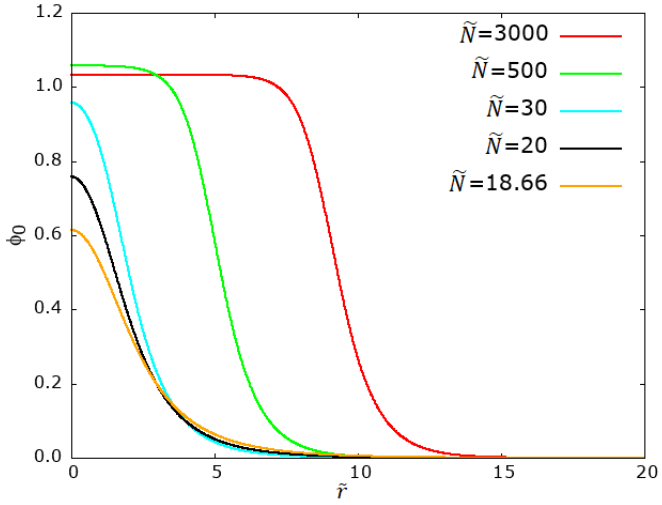

FIG. 1: Ground state wave function of a self-bound droplet as a function of the radial coordinate $\tilde{r}$ for different values of $\tilde{N}$.

B. Ground state: Gaussian ansatz

It is not possible to obtain self-bound droplets for values of $\tilde{N} < 18.65$, even numerically the program can't converge. Since we consider spherically symmetric quantum droplets, we can use a Gaussian ansatz for the ground state to further explore this limit [8]:

$$\phi_0(r) = \frac{\sqrt{N}}{\pi^{3/4}\sigma^{3/2}}\exp\left[-\frac{r^2}{2\sigma^2}\right], \tag{5}$$

where the width σ is the variational parameter, and N and r correspond to the variables $\tilde{N}$ and $\tilde{r}$ described in Sect. II. To simplify the notation, from now on, we will use the dimensionless variables in section II without the tilde symbol.

Let us consider first the general case of a system with an external harmonic potential, with ω_0 the dimensionless trapping frequency. The energy of the droplet is:

$$\mathcal{E}_{\text{TOT}} = \int_0^\infty d\mathbf{r}\left[\phi_0^*(r)\left(-\frac{1}{r}\frac{\partial\phi_0}{\partial r} - \frac{1}{2}\frac{\partial^2\phi_0}{\partial r^2}\right) + \right.$$

$$\left. + \frac{1}{2}\omega_0^2\,r^2\,\phi_0^2 - \frac{3}{2}|\phi_0|^4 + |\phi_0|^5\right]. \tag{6}$$

Using the variational ansatz (5) in Eq. (6), it yields:

$$\frac{\mathcal{E}_{\text{TOT}}}{N} = 4\pi\left[\frac{3}{16\pi\sigma^4} - \frac{3N\sqrt{2}}{32\pi^{5/2}\sigma^3} + \frac{\sqrt{10}N^{3/2}}{50\pi^{13/4}\sigma^{9/2}}\right] + \frac{3}{4}\omega_0^2\sigma^2\,. \tag{7}$$

By minimizing this energy we can obtain a relation between ω_0, N, and the variational parameter σ:

$$\omega_0^2 = \frac{1}{\sigma^4} - \frac{3N\sqrt{2}}{4\pi^{3/2}\sigma^5} + \frac{3N^{3/2}}{(5/2)^{3/2}\pi^{9/4}\sigma^{13/2}}\,. \tag{8}$$

For a given ω_0 and N, the value of the variational parameter shall be obtained numerically.

For a self-bound quantum droplet, without trapping potential $\omega_0 = 0$, there is a range for the number of atoms where the system is metastable. Fig. 2 shows that this range is given by $N \in [N_c, N_m]$. N_m is the value of N where the global energy minimum becomes a local minimum with positive energy. Particles can tunnel into free space and ultimately reach zero energy at infinity. N_c is the value of N where the minimum disappears. For values of N smaller than N_c, the kinetic energy per particle becomes dominant in front of the mean-field and beyond-mean-field energies, breaking the balance and provoking instability [8]. The values for N_m and N_c can be obtained analytically using the Gaussian ansatz, which provides a good approximation with respect to the numerical values.

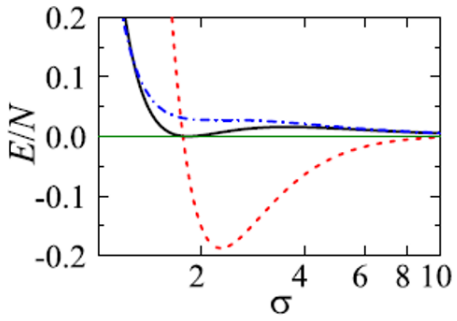

FIG. 2: Energy per particle as a function of σ when $N = N_c$ (blue line), $N = N_m$ (black line), and $N = 100$ (red line) [8].

The lower threshold number N_c is given by $\partial^2(\mathcal{E}_{\mathrm{TOT}}/N)/\partial\sigma^2 = 0$. The calculation of this derivative, by using the expression in Eq. (8), leads to:

$$N_c^{1/2} = \frac{40\sigma^{3/2}\pi^{3/4}}{2^{9/2}\sqrt{10}}\,. \tag{9}$$

Given that $\sigma \approx 1.03$ [8], it follows $N_c = 19.62$. The numerical result is $N_c = 18.65$, which is close to the lowest value of $\tilde{N}$ represented in Fig. 1. The upper threshold N_m, can be calculated by imposing that the total energy is zero which leads to $N_m = 24.03$. However, the Gaussian variational ansatz does not give a good approximation of the density profile of the droplet, since it does not predict the flat-top shape (saturation) of the droplet for large particle numbers.

III. THE BOGOLIUBOV-DE GENNES APPROXIMATION

The elementary excitations or normal modes of a self-bound droplet can be obtained by linearizing the time-dependent extended GPE (2). Within the Bogoliubov-de Gennes approximation [9], we assume small oscillations of the wave function around the stationary solution, ϕ_0, as:

$$\phi(\mathbf{r},t) = [\phi_0(\mathbf{r}) + \delta\phi(\mathbf{r},t)]\, e^{-i\mu t/\hbar}\,, \tag{10}$$

where μ is the chemical potential. Since we will focus on excitations with an energy $\hbar\omega$ around the ground state, we can write:

$$\delta\phi(\mathbf{r},t) = u(\mathbf{r})\, e^{-i\omega t} + v^*(\mathbf{r})\, e^{i\omega t}\,, \tag{11}$$

where ω is the oscillation frequency, and u and v are the components characterizing the Bogoliubov transformation. Notice that there is no loss of generality taking the complex conjugate function $v^*(\mathbf{r})$. Introducing this ansatz in Eq. (2) and retaining terms up to first order in u and v, we find three equations. The first one is the extended GPE for the ground state wave function ϕ_0, Eq. (4), while $u(\mathbf{r})$ and $v(\mathbf{r})$ obey two coupled Bogoliubov equations. Defining the normal mode as $(u(\mathbf{r}), v(\mathbf{r}))$, these coupled equations allow us to find the eigenfrequencies ω as the spectrum of excitations. It can be seen more clearly when the Bogoliubov equations are written in the matrix form:

$$\begin{pmatrix} -\mu - \frac{1}{2}\nabla^2 - 6\phi_0^2 + \frac{25}{4}\phi_0^3 & -3\phi_0^2 + \frac{15}{4}\phi_0^3 \\ -3\phi_0^2 + \frac{15}{4}\phi_0^3 & -\mu - \frac{1}{2}\nabla^2 - 6\phi_0^2 + \frac{25}{4}\phi_0^3 \end{pmatrix} \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix}. \tag{12}$$

All resulting frequencies must be real as can be seen by taking the two Eqs. (12), denoting the upper one by (12.1) and the lower one by (12.2), and performing the following calculations: $[u^*\cdot(12.1) - v\cdot(12.2)^* - u\cdot(12.1)^* + v^*\cdot(12.2)]$. This yields an expression that once integrated on both sides gives place to [9]:

$$(\omega - \omega^*) \int d\mathbf{r}\, \left(|u|^2 - |v|^2\right) = 0\,, \tag{13}$$

where the integral doesn't vanish. Moreover, generalizing the above procedure, it is straightforward to see that two solutions with different frequencies, $\omega_i \neq \omega_j$, fulfill $(\omega_i - \omega_j^*) \int d\mathbf{r}\, (u_i^* u_j - v_i^* v_j) = 0$. Therefore, they must satisfy the ortogonality relation $\int d\mathbf{r}\, (u_i^* u_j - v_i^* v_j) = 0$.

Additionally, when a numerical solution of an oscillation frequency takes a complex value, the system presents a dynamic instability [9]. This can be understood as fol-

lows: if $\omega \in \mathrm{C}$, $\omega = \omega_R + i\,\omega_I$ with $\omega_R, \omega_I \in \mathrm{R}$. Then

$$\delta\phi(\mathbf{r},t) = u(\mathbf{r})\, e^{-i\omega_R t}\, e^{\omega_I t} + v^*(\mathbf{r})\, e^{i\omega_R t} e^{-\omega_I t}\,.$$

This means that for large times, when $t \to \infty$, the exponential $e^{\omega_I t} \to \infty$ and $\delta\phi$ diverges. The latter denotes that the system becomes unstable.

The excited states can be better understood in the second quantization formalism. Starting with the many-body Hamiltonian for a weakly interacting BEC in second quantization up to second-order terms on the creation and annihilation operators,

$$\begin{aligned} H \;=\; & \frac{gN^2}{2V} + \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \\ & + \frac{1}{2} gn \sum_{\mathbf{p}\neq 0} \left[2\hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{-\mathbf{p}} + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} + \frac{mgn}{p^2} \right], \end{aligned} \tag{14}$$

where $\hat{a}^\dagger_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}$, are the creation and annihilation operators of a particle with momentum $\mathbf{p}$, respectively. The density is $n = N/V$, with N the number of particles and V the volume.

The previous Bogoliubov equations can be obtained from Eq. (14) by using the Bogoliubov transformations [10]:

$$\hat{a}_{\mathbf{p}} = u_{\mathbf{p}} \hat{b}_{\mathbf{p}} + v^*_{-\mathbf{p}} \hat{b}^\dagger_{-\mathbf{p}} \tag{15}$$

$$\hat{a}^\dagger_{\mathbf{p}} = u^*_{\mathbf{p}} \hat{b}^\dagger_{\mathbf{p}} + v_{-\mathbf{p}} \hat{b}_{-\mathbf{p}}\,. \tag{16}$$

Writing the operators $\hat{b}^\dagger_{\mathbf{p}}$ and $\hat{b}_{\mathbf{p}}$ in terms of the aforementioned creation and annihilation operators, the former turn out to be a superposition of the latter. In other words, $\hat{b}^\dagger_{\mathbf{p}}$ and $\hat{b}_{\mathbf{p}}$ are a superposition of states with a different number of particles, therefore, they are quasi-particle operators.

More interestingly, the Hamiltonian can be expressed in terms of these new operators in a much simpler and intuitive way [10]:

$$H = E_0 + \sum_{\mathbf{p}} \epsilon(p)\, \hat{b}^\dagger_{\mathbf{p}} \hat{b}_{\mathbf{p}} \tag{17}$$

$$E_0 = \frac{gN^2}{2V} + \frac{1}{2} \sum_{\mathbf{p}\neq 0} [\epsilon(p) - gn - \frac{p^2}{2m} + \frac{m(gn)^2}{p^2}]\,, \tag{18}$$

where E_0 is the energy of the ground state, $\epsilon(p) = \sqrt{(v_s p)^2 + (p^2/(2m))^2}$ is the dispersion relation of the elementary excitations of the system, and $v_s = \sqrt{gn/m}$ is the speed of sound.

At zero temperature, all the bosons of a non-interacting bosonic system (ideal Bose gas) occupy the same single-particle state, and the BEC is formed by all the particles. However, in a weakly interacting bosonic system, the presence of interactions is responsible for a small depletion of the condensate. This phenomenon is called quantum depletion and produces a small reduction in the number of particles of the BEC. The chemical potential, defined as follows, is responsible for this phenomenon since it is the necessary energy for a particle to escape the ground state of the condensate.

$$\mu = \frac{\partial E_0}{\partial N} = gn \left(1 + \frac{32}{3\sqrt{\pi}} \sqrt{n a_s^3} \right). \tag{19}$$

Since E_0 includes the LHY correction, the above expression is the correction to the chemical potential of the extended GPE.

The number of particles out of the condensate that are at excited states can be calculated as [11]:

$$N_{\mathbf{p}} \equiv \langle \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} \rangle = \sum_{\mathbf{p}\neq 0} v^2_{\mathbf{p}}\,. \tag{20}$$

A. Numerical solution of the Bogoliubov equations

To facilitate the solving of the coupled Bogoliubov equations (12), it is useful to write $u(\mathbf{r})$ and $v(\mathbf{r})$ in terms of two auxiliary functions $\psi^\pm(\mathbf{r}) = u(\mathbf{r}) \pm v(\mathbf{r})$ [8].

Defining the ground state potential as $V_{\mathrm{gs}}(\mathbf{r}) = \left(-3\phi_0^2 + \frac{5}{2}\phi_0^3\right)$ and $f(\mathbf{r}) = 2\left(-3\phi_0^2 + \frac{15}{4}\phi_0^3\right)$, equations (12) read:

$$\left(-\frac{1}{2}\nabla^2 + V_{\mathrm{gs}}(\mathbf{r}) - \mu \right) \psi^+(\mathbf{r}) + f(\mathbf{r}) \psi^+(\mathbf{r}) = \omega \psi^-(\mathbf{r}) \tag{21}$$

$$\left(-\frac{1}{2}\nabla^2 + V_{\mathrm{gs}}(\mathbf{r}) - \mu \right) \psi^-(\mathbf{r}) = \omega \psi^+(\mathbf{r})\,. \tag{22}$$

These equations can be solved by expanding the auxiliary functions in a new basis: $\psi^\pm(\mathbf{r}) = \sum_\alpha c^\pm_\alpha \psi_\alpha$. The basis set can be obtained through:

$$\left(-\frac{1}{2}\nabla^2 + V_{\mathrm{gs}}(\mathbf{r}) \right) \psi_\alpha = \epsilon_\alpha \psi_\alpha\,. \tag{23}$$

Substituting the auxiliary wave functions with their respective superposition in Eqs. (21) and (22), multiplying by the complex conjugate of the basis wave functions, and integrating in space leads to:

$$(\epsilon_\alpha - \mu)\, c^-_\alpha = \omega\, c^+_\alpha \tag{24}$$

$$(\epsilon_\alpha - \mu)\, c^+_\alpha + \sum_\beta c^+_\alpha \int \psi^*_\beta\, f(\mathbf{r})\, \psi_\alpha\, d\mathbf{r} = \omega\, c^-_\alpha\,. \tag{25}$$

Inserting Eq. (24) into (25) gives place to an algebraic system of equations. Diagonalizing this system, we can obtain the eigenvalues corresponding to ω^2, being ω the frequency of the excitations, and the eigenstates corresponding to the coefficients c^-_α. The algebraic system reads:

$$c^-_\alpha (\epsilon_\alpha - \mu)^2 + (\epsilon_\alpha - \mu) \sum_\beta c^-_\alpha \int \psi^*_\beta\, f(\mathbf{r})\, \psi_\alpha\, d\mathbf{r} = \omega^2 c^-_\alpha\,. \tag{26}$$

The coefficients c_α^+ can be obtained from Eq. (24).

Fig. 3 shows the results for the lowest monopole mode, the breathing mode, which is the excitation with the lowest energy with $l = 0$, being l the angular momentum of the modes. The numerical result obtained, $\omega = 0.198$, is in perfect agreement with Refs. [2, 8].

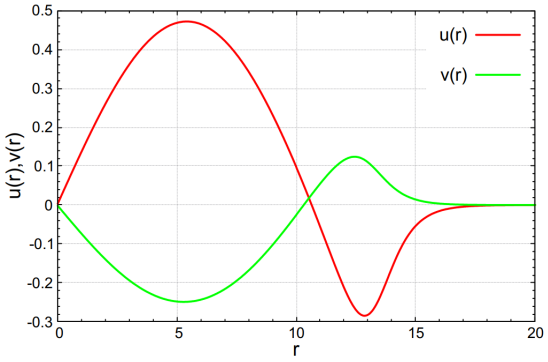

FIG. 3: Reduced radial part of the Bogoliubov functions $u(r)$ and $v(r)$ of the breathing mode for $N = 10000$.

There are two types of modes when it comes to the excitations of the droplet: the bulk mode and the surface mode. The bulk mode spreads through the whole droplet while the surface mode only does so at the surface using the surface tension to propagate [8]. In Fig. 3 it can be seen that the breathing mode is a bulk mode because the perturbation is present at the core of the droplet.

Furthermore, it is important to note that these discrete modes only exist below the particle emission threshold given by $-\mu$ [8].

When the excitation spectrum is located within the continuum region (above the particle emission threshold), the droplet experiences what is called a self-evaporation process. During this process, the droplet loses atoms that tunnel into the vacuum until its energy is below the threshold and it can sustain the collective modes.

In addition, the droplet also experiences three-body losses that continuously steer the system away from equilibrium, ultimately leading to depletion. Generally, three-body losses are dominant in front of the self-evaporation process at the initial stages of the evolution of a quantum droplet. However, it was discovered that there is a range of parameters for which the densities are lower and, thus, the lifetime of the droplet is larger and self-evaporation can take place [12].

Without the presence of three-body losses, the evolution of a droplet gives place to two different scenarios. When the energy is within the continuum region, the droplet experiences self-evaporation and presents damped oscillations (damped monopole mode). On the contrary, if the droplet's energy is below the particle emission threshold, it presents sinusoidal oscillations given by the existence of the monopole mode [8].

IV. SUMMARY AND CONCLUSIONS

Self-bound droplets can be stabilized by a repulsive beyond mean-field correction, the LHY term, which stems from quantum fluctuations and counterbalances the attractive mean-field interaction forces of the droplet.

Moreover, given the spherical symmetry of the droplet, we can consider the Gaussian ansatz approach for the ground state. It can be used to calculate the range of particle numbers within which the system is metastable, but it does not give a good approximation of the density profile because it doesn't predict the flat-top shape of the droplet for large particle numbers.

The excited states of the droplet can be studied through the Bogoliubov-de Gennes approximation. The Bogoliubov equations have been solved numerically to study the first excited state with the lowest energy, the breathing mode. As can be seen from the results, it is a bulk mode since the perturbation starts at the center of the droplet.

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