

Oscillations of squeezed Bose-Bose quantum droplets

Korda, Marko

Master's thesis / Diplomski rad (sveučilišni)

2025

Degree Grantor / Ustanova koja je dodijelila akademski / stručni stupanj: **University of Split, Faculty of Science / Sveučilište u Splitu, Prirodoslovno-matematički fakultet**

Permanent link / Trajna poveznica: <https://um.nsk.hr/um:nbn:hr:166:601812>

Rights / Prava: [Zaštićeno autorskim pravom.](#) / [In copyright.](#)

Download date / Datum preuzimanja: **2026-09-07**



Repository / Repozitorij:

[Digital Repository of Faculty of Science in Split / Digitalni repozitorij Prirodoslovno-matematičkog fakulteta u Splitu](#)



Dabar

University of Split
Faculty of Science

Oscillations of squeezed Bose-Bose quantum droplets

Master thesis

Marko Korda

Split, September 2025

Temeljna dokumentacijska kartica

Sveučilište u Splitu
Prirodoslovno–matematički fakultet
Odjel za fiziku
Ruđera Boškovića 33, 21000 Split, Hrvatska

Diplomski rad

Oscilacije stisnutih Bose-Bose kvantnih kapljica

Marko Korda

Sveučilišni diplomski studij Fizika; smjer: Računarska fizika

Sažetak:

Kvantne Bose-Bose kapljice, jedinstveno samovezано stanje stabilizirano kvantnim fluktuacijama, su ključan poligon za proučavanje višestruke fizike. Međutim, njihove oscilacije u anizotropnim zamkama nisu još u potpunosti razjašnjene. Ovaj rad numerički istražuje kolektivne oscilacije kvantnih kapljica, te njihovo ponašanje uz snažno stiskanje duž jedne osi. Numerički izračuni su provedeni korištenjem teorije funkcionala gustoće, uz energijski funkcional izveden iz rezultata dobivenih u kvantnoj Monte Carlo simulaciji. Oscilacijski spektri su dobiveni za razne veličine kapljica i jačine stiskanja, za monopolni mod (mod disanja) te kvadrupolni mod. Analizom je utvrđeno da stiskanje značajno snižava frekvencije oscilacija i kritični broj atoma potreban za stabilnu kapljicu. Kvadrupolni modovi su pokazali bolju stabilnost u manjim kapljicama, dok su modovi disanja pokazali izraženiju ovisnost o jačini stiskanja. Također, usporedbom sa standardnom teorijom srednjeg polja uz Lee-Huang-Yang korekciju, utvrđeno je da korekcije višeg reda, osnažene stiskanjem, značajnije utječu na mod disanja. Ovi zaključci potvrđuju da su stisnute kapljice obećavajuć sustav za buduće eksperimente.

Ključne riječi: Bose-Bose mješavine, teorija funkcionala gustoće, kvantne kapljice, mod disanja, kvadrupolni mod

Rad sadrži: V stranica s općim podacima, 51 stranicu, 21 sliku, 4 tablice, 37 literaturnih navoda.

Mentor: prof. dr. sc. Leandra Vranješ Markić, *Prirodoslovno-matematički fakultet u Splitu*

Povjerenstvo za ocjenu i obranu diplomskog rada:

prof. dr. sc. Leandra Vranješ Markić, *Prirodoslovno-matematički fakultet u Splitu*

izv. prof. dr. sc. Martina Požar, *Prirodoslovno-matematički fakultet u Splitu*

izv. prof. dr. sc. Petar Stipanović, *Prirodoslovno-matematički fakultet u Splitu*

Datum obrane: 25. 09. 2025.

Rad je napisan na engleskom jeziku i pohranjen u repozitoriju Prirodoslovno–matematičkog fakulteta u Splitu, koji je dio nacionalnog repozitorskog sustava Dabar.

Basic documentation card

University of Split
Faculty of Science
Department of Physics
Ruđera Boškovića 33, 21000 Split, Croatia

Master thesis

Oscillations of squeezed Bose-Bose quantum droplets

Marko Korda

University graduate study Physics, specialization in Computational Physics

Abstract:

Quantum Bose-Bose droplets, a unique self-bound state stabilized by quantum fluctuations, are a key playground for studying many-body physics. However, their oscillating behaviour in anisotropic traps is not yet fully understood. This thesis numerically explores the collective oscillations of these droplets, and their behaviour under strong confinement along one axis. The numerical calculations were performed using the Density Functional Theory, with the energy functional derived from data obtained by the Quantum Monte Carlo simulations. Oscillation spectra were obtained for various droplet sizes and confinement strengths, for both the breathing (monopole) mode and the quadrupole mode. Our analysis reveals that squeezing significantly lowers both the oscillation frequencies and the critical atom number required for a stable droplet. While quadrupole modes exhibit greater stability in smaller droplets, the breathing mode shows a more pronounced dependence on confinement strength. Also, a comparison with standard mean-field plus Lee-Huang-Yang (MF+LHY) theory shows that beyond-LHY effects, enhanced by the confinement, have a much greater impact on the breathing mode. These findings establish that squeezed droplets make a highly promising system for future experimental efforts.

Keywords: Bose-Bose mixtures, density functional theory, quantum droplets, breathing mode, quadrupole mode

Thesis contains: V general information pages, 51 pages, 21 figures, 4 tables, 37 references.

Supervisor: Prof. Dr. Leandra Vranješ Markić, *Faculty of Science in Split*

Thesis defence and evaluation committee:

Prof. Dr. Leandra Vranješ Markić, *Faculty of Science in Split*
Assoc. Prof. Dr. Martina Požar, *Faculty of Science in Split*
Assoc. Prof. Dr. Petar Stipanović, *Faculty of Science in Split*

Defence date: September 25, 2025

The thesis is written in English and archived in the repository of the Faculty of Science, University of Split, which is part of the national repository system DABAR.



This thesis was completed in Split in 2025, as part of the Croatian Science Foundation's project IP-2022-10-6144 "Exploring quantum fluctuations in cold atom systems" (EQUAFLU) under the supervision of Prof. Dr. Leandra Vranješ Markić. Master thesis was submitted for evaluation to the Department of Physics of the University of Split, Faculty of Science.

Declaration of Authorship

I declare, with full material and moral responsibility, that I have independently written the thesis titled Oscillations of squeezed Bose-Bose quantum droplets under the supervision of Prof. Dr. Leandra Vranješ Markić. In the thesis, I have applied scientific research methodology and used literature listed at the end of the thesis. The insights, opinions, conclusions, theories, and principles of others that I have directly quoted or paraphrased in the thesis have been cited in the usual, standard manner and linked to the corresponding bibliographic sources.

Student

Marko Korda

Contents

1	Introduction	1
2	Theory overview	4
2.1	Single component Bose gas	4
2.1.1	Bogoliubov theory	4
2.1.2	Lee-Huang-Yang energy	6
2.1.3	Density functional theory	6
2.1.4	Numerically solving GPE-like equations	8
2.2	Mixtures of Bose gases	9
2.2.1	Stability of a Bose-Bose mixture	10
2.2.2	LHY energy for Bose-Bose mixtures	12
2.2.3	Quantum droplets	12
3	Methods	14
3.1	QMC Density Functional	14
3.2	Multipole moments	15
3.3	Sum rules	16
3.4	Chemical potential	17
3.5	Simulation procedure	18
4	Study of non-squeezed Bose-Bose quantum droplets	20
4.1	Simulation parameters	21
4.2	Results	23
5	Study of squeezed Bose-Bose quantum droplets	27
5.1	Simulation parameters	28
5.2	Breathing mode	32
5.3	Quadrupole mode	35
5.4	Comparison with MF+LHY approach	38
5.5	Comparison between squeezing strengths	41
6	Conclusion	43
7	Bibliography	44
A	Graphs	48

1 Introduction

Quantum particles fall into two categories depending on the behaviour under interchange of two particles and corresponding statistics: bosons and fermions. Fermions follow the Pauli exclusion principle, which states that no more than one fermion can occupy the same quantum state. This restriction underlies the complex structure of matter, most importantly, electronic shells in atoms which enables molecules, chemical reactions and, therefore, practically everything we see. On the other hand, no such limitations exist for bosons, enabling them to occupy the same quantum state in macroscopic numbers.

At the low enough temperature, bosons accumulate in the lowest energy state, giving rise to the new state of matter: Bose-Einstein condensate (BEC), a macroscopic quantum state where all particles share the same wavefunction. This idea was first predicted by Albert Einstein's work in 1925 [1], where he predicted a phase transition during which, at some critical temperature T_C , bosons start to condense at the lowest energy state. When the absolute zero is approached, all bosons in the system are in the condensate, making macroscopic wavefunctions possible to achieve.

The first experimental realisation of Bose-Einstein condensation in alkali vapours was achieved in 1995, making a milestone in atomic physics. Two groups accomplished this breakthrough independently: E. A. Cornell and C. E. Wieman at the University of Colorado created a condensate of rubidium-87 atoms [2], while W. Ketterle and his team at the Massachusetts Institute of Technology (MIT) realized condensation using sodium [3]. These experiments provided the first direct observation of macroscopic quantum phenomena in dilute atomic gases. For this breakthrough, Cornell, Wieman and Ketterle were awarded the Nobel Prize in Physics in 2001.

With the existence of BECs firmly established, the focus of the field shifted from creation to characterization and manipulation. A key experimental development in this pursuit was the usage of Feshbach resonances [4], which allow for the precise tuning of interaction strength between atoms simply by changing an external magnetic field. This high level of control turned ultracold atoms into a versatile quantum playground. On the theoretical front, there was a need for a robust descriptive framework, leading to the widespread adoption of the mean-field approach for these weakly interacting systems.

The standard BEC is a very dilute gas, making the mean-field approach suitable for exploring the theoretical framework. In the mean-field theory we assume all particles to occupy the same single-particle quantum state ($k = 0$). This approach results in the famous Gross-Pitaevskii equation [5, 6], which is essentially an effective nonlinear Schrödinger equation. It captures collective dynamics, ground state properties and excitations of weakly interacting BECs. When the density increases, first correction to the mean-field theory needs to be introduced.

This was first rigorously quantified by T. D. Lee, K. Huang and C. N. Yang in 1957 [7, 8], who derived the analytical expression for the leading-order correction to the energy of a dilute Bose gas, which is known as the Lee-Huang-Yang (LHY) correction. In a single-component Bose gas, mean-field interaction dominates as the corrections are almost negligible. However, in the mixtures of two BECs with interspecies attraction and intraspecies repulsion, D. Petrov predicted [9] a significant manifestation of beyond mean-field effects. A particularly striking discovery is the formation of quantum Bose-Bose droplets which are self-bound states stabilized by quantum fluctuations (the LHY correction) that counteract the mean-field attraction. In order for them to be stable, their number of atoms has to be above some critical number, and in that case the binding energy is negative.

Soon after Petrov's theoretical predictions, experimental groups confirmed the formation of droplets in both dipolar and Bose-Bose mixtures. The first observation of quantum droplets was reported in dipolar condensates of dysprosium atoms by H. Kadau et al. in 2016 [10]. Shortly after, C. Cabrera et al. [11] and Semeghini et al. [12] realized quantum droplets in potassium mixtures, directly confirming Petrov's predictions. These groundbreaking experiments established the crucial role of beyond-mean-field effects in ultracold gases.

Once a novel state of matter like a quantum droplet is realized, a primary experimental and theoretical goal is to characterize its fundamental properties. One of the most powerful, non-destructive methods for this is the study of its collective excitations. By slightly perturbing the droplet and observing its following oscillations, one can directly probe its equation of state, which dictates properties of interest. These collective modes, such as the monopole (breathing) mode and the quadrupole mode, act as the fingerprints of the system. Their oscillation frequencies are very sensitive to the delicate balance between the attractive mean-field energy and the repulsive beyond-mean-field corrections. Early experiments on droplet excitations in spherically symmetric traps provided stunning quantitative verification of the LHY theory [11], as well as beyond-LHY effects including oscillations [13, 14], solidifying our understanding of these self-bound states.

However, the physics of quantum droplets becomes even richer and more complex when the external symmetries are broken. While initial studies focused on droplets in isotropic traps or without external confinement, the frontier of the field now lies in understanding their behaviour under anisotropic confinement. By squeezing using the trapping potential, one can force a dimensional crossover [15, 16]. This crossover from a three-dimensional to a quasi-two-dimensional or quasi-one-dimensional system is not a trivial change, as it fundamentally alters the nature of quantum fluctuations, and therefore, the form of the LHY stabilization term itself. This opens up a fascinating landscape of new phenomena, from the deformation of a single droplet to a train of solitons [17]. It also reduces the critical number of atoms required for a stable self-bound droplet, allowing for easier experimental realisation [11, 18].

The primary objective of this thesis is to investigate the collective oscillations of Bose-Bose

quantum droplets under strong anisotropic confinement, more precisely the strong harmonic trap in the z direction. By employing extensive numerical simulations based on a Quantum Monte Carlo (QMC) derived density functional [19], we aim to find the droplet excitation spectrum for both breathing and quadrupole modes, as a function of confinement strength and the droplet size. Also, the stability of observed oscillation modes will be further investigated, by studying the relation between chemical potential with droplet size and confinement properties. This work seeks to provide a comprehensive understanding of how squeezing affects droplet dynamics and to offer clear and testable predictions for future experiments.

The structure of this thesis is organized as follows: Chapter 2 covers the theory fundamentals, from single to multi-component Bose gases, introducing the mean field theory, Lee-Huang-Yang correction and the density functional theory. In Chapter 3, methods used are covered, from construction of the QMC density functional to the general simulation procedure. In Chapter 4, the study of the non-squeezed droplets is performed and compared against known results from literature to confirm the simulation validity. In Chapter 5, the focus shifts to the study of squeezed droplets, presenting the new results and the discussion. Finally, Chapter 6 concludes the thesis and gives the summary of the results.

2 Theory overview

In this Chapter, short theory overview will be made. It is mainly based on the book from Lev Pitaevskii and Sandro Stringari [20], and the book from C. J. Petchick and H. Smith [21], with parts also taken from Viktor Cikojević's doctoral thesis [22]. First subsection is a brief overview of the basic Bose gas theory, including mean-field and Lee-Huang-Yang approaches, and also introducing the idea of density functional theory. Second subsection will add another type of bosons to the mixture and study Bose-Bose mixtures, arriving on introduction of self-bound Bose-Bose quantum droplets which are the main focus point of this thesis.

2.1 Single component Bose gas

2.1.1 Bogoliubov theory

When there is a system composed of N identical quantum particles of mass m , it obeys the Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)}{\partial t} = \hat{H} \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N), \quad (2.1)$$

with the Hamiltonian given by

$$\hat{H} = \sum_{i=1}^N \left\{ -\frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i) \right\} + \sum_{i < j}^N V_{\text{pair}}(\mathbf{r}_i - \mathbf{r}_j), \quad (2.2)$$

where $V_{\text{ext}}(\mathbf{r})$ is the external potential and V_{pair} is the interaction potential between the two particles. We can write the Hamiltonian in the second-quantization formalism [23]

$$\begin{aligned} \hat{H} = & \int d^3r \hat{\Psi}^\dagger(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right\} \hat{\Psi}(\mathbf{r}) \\ & + \frac{1}{2} \int d^3r \int d^3r' \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}), \end{aligned} \quad (2.3)$$

where $\hat{\Psi}$ is the field operator

$$\hat{\Psi}(\mathbf{r}) = \sum_i \psi_i(\mathbf{r}) \hat{a}_i, \quad (2.4)$$

and $\psi_i(\mathbf{r})$ is the i -th single-particle state, while $\hat{a}_i$ and $\hat{a}_i^\dagger$ are annihilation and creation operators. For particles that follow Bose-Einstein statistics, commutation relations are $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$ and $[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$, and their expectation values are [24]

$$\langle \hat{a}_k^\dagger \hat{a}_k \rangle = N_k, \quad (2.5)$$

where N_k is the occupation number of the k -th state. At near absolute zero temperatures and weak interactions, excited states in Bose systems are barely populated, therefore to a first approximation we can replace the field operator with its average value [24, 25]

$$\hat{\Psi}(\mathbf{r}) \rightarrow \psi = \langle \hat{\Psi} \rangle \approx \psi_0(\mathbf{r}), \quad (2.6)$$

where $\psi_0 = \sqrt{\rho_0}$ is the wavefunction of the condensate, with ρ_0 being the number density of the condensate. In a real system, not all particles are in the condensate. This is due to ground state being mixed with excited states because of the two-body interaction. It can be shown [21] that the depletion of the condensate is

$$\frac{\rho_0}{\rho} = 1 - \frac{8}{3\sqrt{\pi}} \sqrt{\rho a^3}, \quad (2.7)$$

with ρ being a total density and a the s -wave scattering length. It can be seen that the gas parameter ρa^3 has a role of a perturbative parameter of the theory. Experimentally observed, usually, this parameter is of the magnitude order of 10^{-5} , therefore the depletion of the condensate is around one percent.

From the equation of motion for $\hat{\Psi}$

$$i\hbar \frac{\partial \hat{\Psi}}{\partial t} = [\hat{\Psi}, \hat{H}], \quad (2.8)$$

and the Bogoliubov replacement (Eq. (2.6)), the equation of motion for ψ is

$$\begin{aligned} i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = & \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right\} \psi(\mathbf{r}, t) \\ & + \int d^3 r' \psi^*(\mathbf{r}', t) V_{\text{int}}(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}', t) \psi(\mathbf{r}, t). \end{aligned} \quad (2.9)$$

Interaction potential usually has a complicated form, but generally it can be broken down to short-range hard-core repulsive part and a long-range Van der Waals tail which is attractive and diminishes as $\propto r^{-n}$ at large distances. When the incident wave-vector k of the interparticle collisions is small, and the mean interparticle distance is significantly larger than the typical potential range, we can replace interparticle potentials with the effective potential

$$V_{\text{int}}(\mathbf{r} - \mathbf{r}') \rightarrow V_{\text{eff}}(\mathbf{r} - \mathbf{r}') = \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r} - \mathbf{r}'), \quad (2.10)$$

where a is the s -wave scattering length, which determines the strength of the potential. When

we use this substitution in the Equation (2.9), we get the Gross-Pitaevskii equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right\} \psi(\mathbf{r}, t) + \frac{4\pi\hbar^2 a}{m} |\psi(\mathbf{r}, t)|^2 \psi(\mathbf{r}, t). \quad (2.11)$$

This equation is not restricted to soft potentials, it generally holds for arbitrary interactions, with the s -wave scattering length a as the relevant interaction parameter. It was derived independently by E. P. Gross [5] and Lev Pitaevskii [6] in 1961 and is the main theoretical tool for dealing with nonuniform dilute Bose gases at very low temperatures. The important peculiarity of the Gross-Pitaevskii equation is its nonlinearity, which arises from the interactions between particles.

We can shortly discuss the limits of applicability of GPE. Firstly, the total atom number must be large enough so the statistical approach holds, thus allowing us to introduce the Bose-Einstein condensation. Second condition requires that the system temperature is low enough and that the interparticle interactions are weak, so we can replace the field operator with the classical field as in Eq. (2.6). Lastly, we are allowed to use GPE only when studying phenomena taking place over distances far greater than the scattering length a .

2.1.2 Lee-Huang-Yang energy

As the density of the condensate increases, higher-order momentum contributions to effective interactions become non-negligible, so we need to account for the condensate depletion. Replacement of the interaction potential with the effective one (Eq. (2.10)) becomes incorrect, as it holds only for very small values of the gas parameter ρa^3 . First correction to the mean-field energy is called the Lee-Huang-Yang (LHY) potential [7, 8]. Ground-state energy per particle of the single-component Bose gas, with incorporated LHY correction, is

$$\frac{E}{N} = \frac{2\pi\hbar^2 a}{m} \rho \left\{ 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} \right\}. \quad (2.12)$$

Correcting the mean-field energy with the LHY term is correct up to $\rho a^3 \approx 10^{-3}$. For higher densities, more scattering parameters are required because the universality in terms of the s -wave scattering length is ended [26, 27]. LHY correction term has been also derived for the non homogeneous Bose gas [28], and confirmed to hold up to $\rho a^3 \approx 10^{-3}$ in a QMC simulation [29].

2.1.3 Density functional theory

Density Functional Theory (DFT) presents an alternative method for tackling many-body problems [30, 31]. The theory is built upon the ground-state particle density, which is defined as

$$\rho(\mathbf{r}) = \int d^3\mathbf{r}_2 \dots d^3\mathbf{r}_N \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N), \quad (2.13)$$

where Ψ is the many-body solution to the Schrödinger equation. This density can be found by minimizing the energy functional, $E[\rho(\mathbf{r})]$, composed of kinetic (T), external potential (V_{ext}), and interaction (V_{int}) energy terms

$$\begin{aligned} E[\rho(\mathbf{r})] &= T[\rho(\mathbf{r})] + V_{\text{ext}}[\rho(\mathbf{r})] + V_{\text{int}}[\rho(\mathbf{r})] \\ &= \langle \Psi | -\frac{\hbar^2}{2m} \nabla^2 | \Psi \rangle + \langle \Psi | V_{\text{ext}} | \Psi \rangle + \langle \Psi | V_{\text{int}} | \Psi \rangle, \end{aligned} \quad (2.14)$$

where $\nabla^2 = \sum_{i=1}^N \nabla_i^2$, $V_{\text{ext}} = \sum_{i=1}^N V_{\text{ext}}(\mathbf{r}_i)$ and $V_{\text{int}} = \sum_{i<j}^N V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|)$. The task of determining the ground-state density and other observables thus becomes a minimization problem with Eq. (2.14). There is one-to-one correspondence between the ground-state density profile $\rho(r)$ and the Hamiltonian of the system making this theory exact in its nature. In practice, however, the exact form of the interaction energy density is unknown and must be approximated, making this theory non-exact in practice. Fortunately, it has been shown [32] that this challenge can be addressed by empirically constructing density functionals from data generated by exact methods, such as diffusion Monte Carlo simulations.

For a system described as a pure condensate, we can implement the Hartree approximation. This involves treating the many-body wavefunction as a product of identical single-particle states

$$\Psi_H(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{i=1}^N \psi(\mathbf{r}_i). \quad (2.15)$$

A crucial assumption is then made for the interaction energy term, expressing it as an integral of an interaction energy density

$$\langle \Psi | V_{\text{int}} | \Psi \rangle = \int d^3r \mathcal{E}_{\text{int}}[\rho], \quad (2.16)$$

where the energy-density term $\mathcal{E}_{\text{int}}(\mathbf{r})$ accounts for all interaction effects. To derive the time evolution of the system, we first need to introduce the Lagrangian L

$$\begin{aligned} L &= \int d^3r \mathcal{L} \\ &= \int d^3r \left[\frac{i\hbar}{2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) - \frac{\hbar^2}{2m} |\nabla \psi|^2 - V_{\text{ext}}(\mathbf{r}) |\psi|^2 - \mathcal{E}_{\text{int}}(\mathbf{r}) \right], \end{aligned} \quad (2.17)$$

and then apply the principle of least action $\delta \int_{t_1}^{t_2} L dt = 0$ which yields a Schrödinger-like equation. When the local density functional is proportional to some power of the density ρ , the resulting equation of motion for ψ is

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}}_{\text{DFT}} \psi = \left\{ -\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}} + \frac{\partial \mathcal{E}_{\text{int}}}{\partial \rho} \right\}. \quad (2.18)$$

This formalism can be directly linked to the results of QMC simulations. The bulk properties of the system can be accurately determined by fitting the numerically calculated energy per particle, E/N . Consequently, the interaction term $\mathcal{E}_{\text{int}}$, can be expressed as [22]

$$\mathcal{E}_{\text{int}} = \frac{E}{N} \rho. \quad (2.19)$$

2.1.4 Numerically solving GPE-like equations

In order to be able to solve Eq. (2.18), firstly, we need to discretize the space domain by making every axis an equally spaced one-dimensional grid. Wavefunction of interest ψ has a value for every point located at the grid intersections. It evolves through time by applying the time-evolution operator at each discretized time step Δt which can be written as

$$\psi(t + \Delta t) = \mathcal{T}(\Delta t) \psi(t), \quad (2.20)$$

where the time-evolution operator $\mathcal{T}$ can be written as

$$\mathcal{T}(\Delta t) = e^{\{-i\hat{\mathcal{H}}_{\text{DFT}}\Delta t/\hbar\}}. \quad (2.21)$$

It is not known analytically, so we approximate it using the Trotter formula. The simplest one is second-order Trotter propagation formula

$$\mathcal{T}(\Delta t) = e^{-i\Delta t V(r')/2\hbar} e^{-i\Delta t \hbar \nabla^2 / 2m} e^{-i\Delta t V(r)/2\hbar} + \mathcal{O}(\Delta t^3). \quad (2.22)$$

Propagators that contain the potential

$$V = V_{\text{ext}}(\mathbf{r}) + \frac{\partial \mathcal{E}_{\text{int}}}{\partial \rho} \quad (2.23)$$

are evaluated in real space, while the middle propagator is evaluated in wave-number space. The whole propagator remains unitary, therefore it preserves the number of particles during the real-time propagation. For obtaining ground-states, we perform time propagation in imaginary time by substituting $\tau = -it/\hbar$. For large enough imaginary-time propagation, only ground-state remains from the wavefunction, since every excited state decays exponentially. The overall

method [22] is presented bellow:

a)

$$\psi_1(\mathbf{r}) = G_1 \cdot \psi(\mathbf{r}, t), \quad (2.24)$$

where

$$G_1 = \exp \left\{ -\frac{1}{2} i \Delta t V / \hbar \right\}, \quad V = V_{\text{ext}}(\mathbf{r}) + \frac{\partial \mathcal{E}_{\text{int}}}{\partial \rho}, \quad \rho = |\psi(\mathbf{r}, t)|^2. \quad (2.25)$$

Here, the operator $(\cdot)$ denotes the element-wise multiplication. The output tensor has the same dimensions as the two tensors to be multiplied, with each grid point (i, j, k) computed as the product of the corresponding elements from the two tensors.

b)

$$\psi_2(\mathbf{r}) = \text{FFT}^{-1} [G_2 \cdot \text{FFT} [\psi_1]], \quad (2.26)$$

where

$$G_2 = \exp \{ -i \Delta t \hbar k^2 / 2m \}. \quad (2.27)$$

The abbreviation FFT stands for Fourier transform, which is used for transition from the r -space to the k -space. In preparation for the next step, we need to return to the r -space which is accomplished by applying inverse Fourier transform denoted by FFT^{-1} .

c)

$$\psi(\mathbf{r}, t + \Delta t) = G_1 \cdot \psi_2(\mathbf{r}), \quad (2.28)$$

where

$$G_1 = \exp \left\{ -\frac{1}{2} i \Delta t V / \hbar \right\}, \quad V = V_{\text{ext}}(\mathbf{r}) + \frac{\partial \mathcal{E}_{\text{int}}}{\partial \rho}, \quad \rho = |\psi_2(\mathbf{r})|^2. \quad (2.29)$$

This last step is very similar to the first, only difference being intermediate wave function $\psi_2(\mathbf{r})$ and the corresponding density ρ being used instead of the initial ones.

2.2 Mixtures of Bose gases

Now, we are going to consider mixtures of two Bose-Einstein condensates. The Hartree wavefunction reads

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{i=1}^{N_1} \psi_1(\mathbf{r}_i) \prod_{j=N_1+1}^N \psi_2(\mathbf{r}_j), \quad (2.30)$$

where N_1 and N_2 are the number of atoms of the first and second component, respectively. Furthermore, $N = N_1 + N_2$ is the total atom number. A general density functional for the two-component quantum Bose-Bose mixture can be written as

$$\begin{aligned} \mathcal{E}[\rho_1, \rho_2] = & \frac{\hbar^2}{2m_1} |\nabla \psi_1(\mathbf{r})|^2 + V_{\text{ext}}^{(1)}(\mathbf{r}) |\psi_1(\mathbf{r})|^2 + \\ & \frac{\hbar^2}{2m_2} |\nabla \psi_2(\mathbf{r})|^2 + V_{\text{ext}}^{(2)}(\mathbf{r}) |\psi_2(\mathbf{r})|^2 + \\ & \mathcal{E}_{\text{int}}[\rho_1, \rho_2], \end{aligned} \quad (2.31)$$

where m_i is the mass of atom from i -th component and $V_{\text{ext}}^{(i)}(\mathbf{r})$ is the external potential applied to the i -th component. In a two-component Bose-Bose mixture, the mean-field energy functional with point interactions is

$$\mathcal{E}_{\text{int}}^{\text{MF}} = \frac{1}{2} g_{11} \rho_1^2 + \frac{1}{2} g_{22} \rho_2^2 + g_{12} \rho_1 \rho_2, \quad (2.32)$$

where $g_{ii} = 4\pi\hbar^2 a_{ii}/m_i$ ($i = 1, 2$), $g_{12} = 2\pi\hbar^2 a_{12}/\mu$ and $\mu = (m_1 m_2)/(m_1 + m_2)$. The corresponding coupled equations for ψ_1 and ψ_2 , the Gross-Pitaevskii equations, are

$$i\hbar \frac{\partial \psi_i}{\partial t} = \left\{ -\frac{\hbar^2}{2m_i} \nabla^2 + V_i(\rho_1, \rho_2) \right\} \psi_i, \quad (2.33)$$

where $i = 1, 2$ and

$$V_i = g_{ii} \rho_i + g_{12} \rho_j, \quad (2.34)$$

with $j \neq i = 1, 2$. Also, $\rho_i = |\psi_i|^2$.

2.2.1 Stability of a Bose-Bose mixture

For a mixture to be stable, the energy must be at a minimum, therefore it must increase for deviations of both densities $\delta\rho_1$ and $\delta\rho_2$. For an infinitesimal density variation, kinetic energy terms can be neglected, so the total energy of a homogeneous Bose-Bose mixture using the mean-field approximation is

$$E = \int d^3r \mathcal{E}_{\text{int}} = \int d^3r \left\{ \frac{1}{2} g_{11} \rho_1^2 + \frac{1}{2} g_{22} \rho_2^2 + g_{12} \rho_1 \rho_2 \right\}. \quad (2.35)$$

A first order variation δE reads

$$\delta E = \int d^3r \left\{ \frac{\partial \mathcal{E}_{\text{int}}}{\partial \rho_1} \delta \rho_1 + \frac{\partial \mathcal{E}_{\text{int}}}{\partial \rho_2} \delta \rho_2 \right\}, \quad (2.36)$$

which vanishes because the number of atoms is conserved $\int d^3r \delta\rho_i = 0$, for $i = 1, 2$. Second-order variation is

$$\delta^2 E = \frac{1}{2} \int d^3r \left\{ \frac{\partial^2 \mathcal{E}_{\text{int}}}{\partial \rho_1^2} (\delta\rho_1)^2 + \frac{\partial^2 \mathcal{E}_{\text{int}}}{\partial \rho_2^2} (\delta\rho_2)^2 + 2 \frac{\partial^2 \mathcal{E}_{\text{int}}}{\partial \rho_1 \partial \rho_2} (\delta\rho_1 \delta\rho_2) \right\}. \quad (2.37)$$

Expanding the integrand to a positive definite square, it reads

$$\begin{aligned} \left(\sqrt{\frac{\partial \mu_1}{\partial \rho_1}} \delta\rho_1 \pm \sqrt{\frac{\partial \mu_2}{\partial \rho_2}} \delta\rho_2 \right)^2 &= \frac{\partial \mu_1}{\partial \rho_1} (\delta\rho_1)^2 + \frac{\partial \mu_2}{\partial \rho_2} (\delta\rho_2)^2 + 2 \delta\rho_1 \delta\rho_2 \frac{\partial^2 \mathcal{E}_{\text{int}}}{\partial \rho_1 \partial \rho_2} \\ &\quad + 2 \delta\rho_1 \delta\rho_2 \left\{ \pm \sqrt{\frac{\partial \mu_1}{\partial \rho_1} \frac{\partial \mu_2}{\partial \rho_2}} - \frac{\partial^2 \mathcal{E}_{\text{int}}}{\partial \rho_1 \partial \rho_2} \right\}, \end{aligned} \quad (2.38)$$

where the chemical potential is $\mu_i = \partial \mathcal{E}_{\text{int}} / \partial \rho_i$, for $i = 1, 2$. Requiring $\delta^2 E > 0$ leads to the conditions

$$\frac{\partial \mu_i}{\partial \rho_i} = g_{ii} \geq 0, \quad (2.39)$$

and

$$\pm \sqrt{\frac{\partial \mu_1}{\partial \rho_1} \frac{\partial \mu_2}{\partial \rho_2}} - \frac{\partial^2 \mathcal{E}_{\text{int}}}{\partial \rho_1 \partial \rho_2} = \pm \sqrt{g_{11} g_{22}} - g_{12} \geq 0. \quad (2.40)$$

Condition shown in Eq. (2.39) is due to the requirement of stability against collapse of each of the components. In case of attractive interactions, when g_{ii} is negative, the system is unstable under variations of density, therefore it is a self bound cluster. For the repulsive interspecies interactions, $g_{12} > 0$, the requirement for stability is obtained for a positive sign in Eq. (2.40), and is

$$g_{12} \leq \sqrt{g_{11} g_{22}}. \quad (2.41)$$

This condition ensures that the density disturbance of any of the two components does not lead to their phase separation. In case of negative sign in Eq. (2.40), when interspecies interactions are attractive, the stability condition is

$$g_{12} \leq -\sqrt{g_{11} g_{22}}, \quad (2.42)$$

so it prevents the formation of a self bound cluster due to the stronger interspecies attraction over geometric average of intraspecies repulsion. When $g_{12} = -\sqrt{g_{11} g_{22}}$, the optimal configuration satisfies $\rho_2 / \rho_1 = \sqrt{g_{11} / g_{22}}$, according to Eq. (2.38). For $g_{12} > -\sqrt{g_{11} g_{22}}$, the ground-state is

either a collapsed state or a dense droplet, depending on the number of atoms.

2.2.2 LHY energy for Bose-Bose mixtures

As mentioned in section 2.1.2, the first energy correction to the mean-field is the Lee-Huang-Yang term, which is derived in [33] for quantum mixtures. It becomes significant as we increase interaction strength and density of the gas, making condensate depletion non negligible. The LHY energy density term is

$$\mathcal{E}_{\text{LHY}} = \frac{8}{15\pi} \left(\frac{m_1}{\hbar^2} \right)^{3/2} (g_{11}\rho_1)^{3/2} f \left(\frac{m_2}{m_1}, \frac{g_{12}^2}{g_{11}g_{22}}, \frac{g_{22}\rho_2}{g_{11}\rho_1} \right), \quad (2.43)$$

where $f(z, u, x)$ is shown in [34]. If we have a mixture of different hyperfine states of the same atoms, for which $m_1 = m_2$ and $z = 1$, it becomes [9]

$$f(1, u, x) = \frac{1}{4\sqrt{2}} \sum_{\pm} \left(1 + x \pm \sqrt{(1-x)^2 + 4ux} \right)^{5/2}. \quad (2.44)$$

For a two-component mixture with $g_{11} \neq g_{22} \neq g_{12}$, the LHY term is given in terms of an integral which solution is not analytically obtainable. Nevertheless, an accurate and effective expression for it was shown in [35], therefore the LHY term for a mixture with approximation $g_{12}^2 = g_{11}g_{22}$, is

$$\mathcal{E}_{\text{LHY}} \simeq \frac{8m_1^{3/2}(g_{11}\rho_1)^{5/2}}{15\pi^2\hbar^3} \left[1 + \left(\frac{m_2}{m_1} \right)^{3/5} \frac{g_{22}\rho_2}{g_{11}\rho_1} \right]^{5/2}. \quad (2.45)$$

2.2.3 Quantum droplets

A mixture with attractive mean-field energy can be balanced with the repulsive LHY energy, resulting in a stable self-bound droplet. This stabilization arises from the interplay between mean-field forces and quantum fluctuations. Dmitri Petrov demonstrated [9] a theoretical explanation of these droplets. Classical mean-field approach does not produce energy that has a minimum, thus we need an extension within LHY theory which modifies total energy so it obtains a distinct, stable global minimum. This can be illustrated easily by numerically evaluating both energies and visualising them in Fig. 1.

In the focus of this thesis are the mixtures with $g_{11} > 0$, $g_{22} > 0$ and $g_{12} < 0$. In other words, mixtures where intraspecies interactions are repulsive and interspecies interactions are attractive, allowing an energy minimum to be possible.

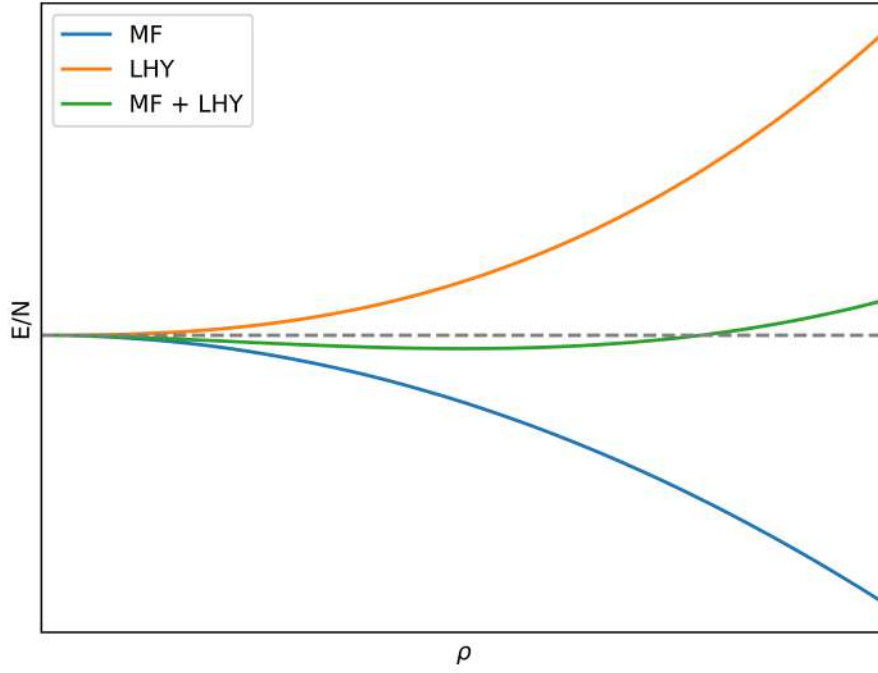


Figure 1: Graphical illustration of the balance between repulsive mean-field (MF) and attractive Lee-Huang-Yang (LHY) interactions which allows for quantum droplet formation. Both the density ρ and energy per particle E/N are in arbitrary units.

3 Methods

In this Section, we will make a brief overview of methods used in this thesis. First, we will explain how to form an energy functional from data obtained by QMC simulation. Also, we will present the sum rule approach for quickly predicting approximate values for peak frequencies. Then, the Liquid Drop Model will be introduced in order to link the chemical potential to the number of atoms, with the aim of establishing a stability threshold. In the end, the simulation procedure will be presented.

3.1 QMC Density Functional

A key step in describing quantum droplets of Bose mixtures is to establish an accurate energy functional that can be applied within the local density approximation. While the mean-field (MF) plus Lee-Huang-Yang (LHY) correction provides an universal and analytic expression, it is derived under the assumption of weak interactions and may become inaccurate in regimes where correlations or finite-range effects are non-negligible. In contrast, quantum Monte Carlo (QMC) simulations, such as the diffusion Monte Carlo (DMC), offer an exact approach within statistical noise that captures the full many-body correlations of the system. The key problem with QMC simulations of a large number of atoms is that they are computationally very expensive, and quickly become intractable as the number of particles increases. To make QMC results usable in practical calculations, they can be parametrized by a compact density functional.

We consider ^{39}K mixtures at the optimal relative atom concentration yielded by the mean field theory [9]

$$N_1/N_2 = \sqrt{a_{22}/a_{11}}. \quad (3.1)$$

For such mixtures, it is shown [22] that the energy per atom in the QMC approach can be written as

$$\frac{E}{N} = \alpha\rho + \beta\rho^\gamma, \quad (3.2)$$

where ρ is the total atom number density. The parameters α , β and γ were determined [18] by fitting to the results obtained by DMC simulation for the model potentials that satisfy the s -wave scattering length and effective range. This parametrization provides an effective density functional that encapsulates beyond-MF effects while remaining computationally tractable. This approach does not yield an universal expression for E/N , as it depends on the value of the applied B , which tunes the interaction strengths. Table 1 shows obtained parameters for three different magnitudes of B . As the magnetic field increases, α becomes less negative while both

Table 1: *Parameters of the QMC density functional for various strengths of the magnetic field B , empirically determined by fitting to the DMC simulation data. These values are taken from [18].*

$B(\text{G})$	α	β	γ
56.230	-0.812	5.974	1.276
56.453	-0.423	8.550	1.373
56.639	-0.203	12.152	1.440

β and γ increase, reflecting the strengthening of repulsive correlations in the mixture. For all the calculations performed throughout this thesis, $B = 56.230$ G will be used.

For the same relative concentration, the MF+LHY energy per particle can be written in similar expression

$$\frac{E/N}{|E_0|/N} = -3 \left(\frac{\rho}{\rho_0} \right) + 2 \left(\frac{\rho}{\rho_0} \right)^{3/2}, \quad (3.3)$$

where E_0/N and ρ_0 are the equilibrium energy per atom and equilibrium density. In contrast to Eq. (3.2), this expression is written in terms of universal quantities and does not depend explicitly on B .

The energy per atom shown in Equation (3.2) allows for introducing, within local density approximation, a density functional whose interacting part is

$$\mathcal{E}_{\text{int}} = \rho \frac{E}{N} = \alpha \rho^2 + \beta \rho^{\gamma+1}. \quad (3.4)$$

This form is directly applicable to studies of droplets in external traps or inhomogeneous geometries, allowing one to capture the beyond-MF correlations encoded in the QMC simulations. A similar construction can be made for the MF+LHY energy functional, where the interaction part can also be expressed as a power series in ρ . The essential distinction is therefore between universality (MF+LHY) and system-specific accuracy (QMC).

3.2 Multipole moments

In this thesis we will focus on two oscillation modes; the breathing mode and the quadrupole mode which are the oscillations of the monopole moment Q_0 and the quadrupole moment Q_2 , respectively.

The monopole moment Q_0 is a measure of the overall size of the system, as it is directly proportional to the mean square radius of the particle distribution. Therefore, oscillations in Q_0 correspond to isotropic expanding and shrinking of the droplet, which appears as "breathing" of the droplet. The quadrupole moment Q_2 measures the anisotropy of the spacial distribution along a chosen axis. A non-vanishing Q_2 indicates an elongated or flattened shape of the droplet

along this axis, and oscillations of Q_2 correspond to transitions between prolate and oblate shapes of the droplet. This is illustrated in Fig. 2.

The discrete definition of the monopole moment Q_0 is

$$Q_0 = \sum_i^N r_i^2, \quad (3.5)$$

where sum is over all atoms in the system, and r_i^2 is the squared distance of particle from the origin of the coordinate system. Similarly, the quadrupole moment is defined as

$$Q_2 = \sum_i^N (3z_i^2 - r_i^2) = \sum_i^N (2z_i^2 - x_i^2 - y_i^2), \quad (3.6)$$

where z is selected as the axis of interest, as the quadrupole moment is defined along some axis. Analogously, Q_2 can be defined along other two axes

$$Q_2^{(x)} = \sum_i^N (3x_i^2 - r_i^2) = \sum_i^N (2x_i^2 - y_i^2 - z_i^2), \quad (3.7)$$

$$Q_2^{(y)} = \sum_i^N (3y_i^2 - r_i^2) = \sum_i^N (2y_i^2 - x_i^2 - z_i^2). \quad (3.8)$$

In our analysis, to excite the droplet, we use a potential of the form

$$V_i = \lambda Q_i, \quad (3.9)$$

where λ is a perturbative parameter of arbitrary choice, and Q_i is the moment which corresponds to the oscillation mode of interest. The choice of perturbation potential V_i ensures coupling to the desired collective mode. Perturbing with V_0 uniformly increases or decreases the radius of the droplet for a small amount. Then, after turning off the perturbation, system exhibits monopole oscillations. Similarly, perturbing with V_2 elongates the droplet along the chosen axis, which excites quadrupole oscillations. The arbitrary parameter λ is a measure of the perturbation strength, and in our calculations is kept small enough so the oscillations remain in harmonic regime.

3.3 Sum rules

When the majority of the multipole strength is in a single narrow peak, it is possible to estimate the peak frequency using the sum rules approach [20, 36]. For the monopole and quadrupole modes, the E_1 energies are

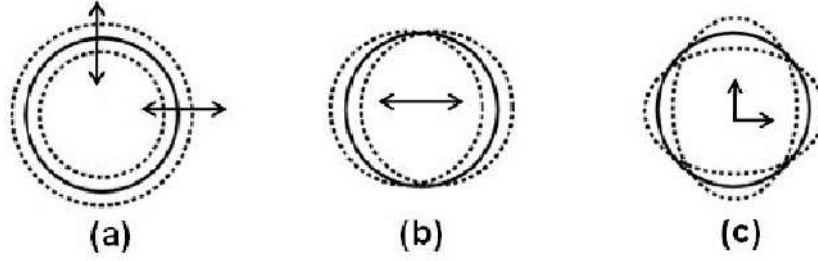


Figure 2: Graphical illustration of different oscillation modes for a spherical droplet. Modes shown are: (a) breathing (monopole) mode, (b) dipole mode and (c) quadrupole mode. Figure taken from [37]

$$E_1(l=0) = -\sqrt{-\frac{4\hbar^2}{m} \frac{\langle r^2 \rangle}{(\partial \langle Q_0 \rangle / \partial \lambda) |_{\lambda=0}}}, \quad (3.10)$$

and

$$E_1(l=2) = -\sqrt{-\frac{8\hbar^2}{m} \frac{\langle r^2 \rangle}{(\partial \langle Q_2 \rangle / \partial \lambda) |_{\lambda=0}}}, \quad (3.11)$$

where λ is the strength parameter of the perturbation in the Hamiltonian.

Results obtained from these formulas will be compared against numerically obtained frequencies to mutually ensure validity of both approaches. However, it must be remembered that these expressions are just an estimation and can not be used as an exact analytical benchmark.

3.4 Chemical potential

It is also needed to study the relation between the chemical potential and the oscillation energy, because the chemical potential plays a crucial role in determining the stability of collective excitations. In general, the chemical potential μ is defined as the energy cost of adding or removing a single particle from the system. For oscillations to be stable, their energy must fall below the absolute value of the chemical potential $|\mu|$. When energy lies above this threshold, then it is energetically favourable to eject atoms from the droplet, making the droplet unstable.

In order to determine how μ depends on the system size, let's introduce the Liquid Drop Model (LDM)

$$E = E_V N + E_S N^{2/3} + E_C N^{1/3} \quad (3.12)$$

which connects energy of the droplet E with the number of atoms N . The first term is known as the volume term, which is proportional to the number of atoms N , i.e. the volume of the droplet. Second term is the surface term, which is a correction to the first term due to surface atoms not

being completely surrounded by atoms, thus not having the same amount of interaction energy. Third term is the curvature term, which accounts for energy that emerges as a result of the droplet curvature.

Model coefficients E_V , E_S and E_C have to be determined by fitting to the data obtained by the simulation. We will write the equation (3.12) in the form

$$\frac{E}{N} = E_V + E_S x + E_C x^2 \quad (3.13)$$

where $x = N^{-1/3}$. This formulation is convenient as we only have to deal with energy per particle, which is of the same order of magnitude across the whole range of N . Also, we need to calculate $\frac{\partial E}{\partial N}$ of the equation (3.12) to obtain

$$\frac{\partial E}{\partial N} = E_V + \frac{2}{3}E_S N^{-1/3} + \frac{1}{3}E_C N^{-2/3} \quad (3.14)$$

where we recognise left side of the equation as the chemical potential μ . This expression shows explicitly how the chemical potential μ depends on the number of atoms in the system N . For very large N , surface and curvature contributions vanish, and $\mu \approx E_V$, which is expected for an infinite homogeneous system. For smaller N , surface and curvature contributions become significant, lowering the binding energy and therefore reducing the stability of oscillations.

By comparing the numerically obtained oscillation energies with the chemical potential, we can easily determine whether a given collective mode is stable against particle emission. This provides a clean way for distinguishing the stable collective oscillations from the decaying modes.

3.5 Simulation procedure

The simulations performed in this thesis follow a systematic three-step procedure which develops a stable ground state, then perturbs it using $V_i = \lambda Q_i$ perturbation potential, and finally evolves the system in real time, extracting dynamical information about the oscillations of interest. It can be decomposed as follows:

a) Ground-state preparation (imaginary-time propagation)

The simulation begins by initialisation of the trial wavefunction, and propagation in imaginary time without the application of the external perturbation. Imaginary-time propagation ensures that all excited states decay exponentially, converging the wavefunction to the ground-state of the system. The output of this step is the wavefunction of the droplet stabilized in the ground energy state. Energy per particle from this step is used for obtaining the LDM coefficients in Eq. (3.13).

b) Stabilization of the perturbed state (imaginary-time propagation)

In the second step, the obtained ground-state wavefunction is loaded and an external perturbative potential $V_i = \lambda Q_i$ is applied, which is chosen to couple specifically to the oscillation mode of interest. For breathing mode this corresponds to the operator Q_0 (Eq. (3.5)), while for quadrupole mode the perturbation is proportional to Q_2 (Eq. (3.6)). The magnitude of the perturbation parameter λ is very small so that the system is only slightly deformed, therefore oscillates harmonically. System is propagated in the imaginary time in order to stabilise the wavefunction in this new, perturbed state. The output of this step is the wavefunction of the droplet, stabilized in the slightly deformed state. We then use outputs from simulations with different values of λ in order to perform the sum rule calculation (Eqs. (3.10) and (3.11)).

c) Real-time propagation and oscillation data extraction

Finally, the external perturbation is removed and the system is propagated in real time, which gives rise to the oscillations of the droplet. During this long-time evolution, we calculate the expectation values of the monopole and quadrupole operators, $\langle Q_0(t) \rangle$ and $\langle Q_2(t) \rangle$, at the regular time intervals. This captures the collective oscillations of the droplet. A Fourier transform of $\langle Q_0(t) \rangle$ and $\langle Q_2(t) \rangle$ is then performed to extract the corresponding frequencies.

Exact details about calculations were discussed earlier in the explanation of Trotter propagation formula.

4 Study of non-squeezed Bose-Bose quantum droplets

In this Chapter, we focus on the study of ordinary three-dimensional non-squeezed Bose-Bose quantum droplets. The main objective of this Chapter is to benchmark and validate our numerical approach before moving to the more intricate squeezed droplets. It will be validated by comparing against the results reported in [22].

In addition, the peak frequencies obtained from the simulations will be compared against the predictions of the sum rule approach (Eqs. (3.10) and (3.11)) to verify them as a good analytical approximation method. Finally, we will employ the Liquid Drop Model (Eq. (3.12)) to empirically determine a relation between the chemical potential μ and the number of atoms N with the aim of developing a practical criterion for determining the stability of the collective oscillations. Such a criterion is of particular importance in determining the critical atom number, where instabilities may set in.

In order to simplify the numerical calculations and avoid dealing with impractical numbers, it is convenient to introduce a system of natural units based on the scattering length a_{11} . This way, all physical quantities can be expressed in dimensionless form, and the SI values can be restored later if needed. We begin by defining the basic length scale as the scattering length a_{11} , which sets the natural unit for sizes and distances. In pair with the particle mass m , it defines the natural energy scale

$$E_0 = \frac{\hbar^2}{2ma_{11}^2}, \quad (4.1)$$

which is set to one in our calculations. We can also define the corresponding natural unit of time

$$t_0 = \frac{2ma_{11}^2}{\hbar}. \quad (4.2)$$

From these base definitions, we derive the corresponding units of all other physical quantities of interest, which are presented in Table 2.

By formulating the problem in this system of natural units, all quantities appearing in the Hamiltonian and in the dynamical equations become dimensionless. This greatly simplifies both numerical simulations and analytical approaches, while ensuring that the physical interpretation of the results remains straightforward. All physical quantities can be easily converted back to the SI units as shown in Table 2, in order to compare the results from the simulations with the real experimental results.

Table 2: Natural units of relevant physical quantities based on the scattering length a_{11} and atom mass m . For reference, SI values of the corresponding units are shown for $B = 56.230$ G.

Physical quantity	Natural unit	SI value
L (length)	a_{11}	$63.648a_0 \approx 3.368 \cdot 10^{-9}$ m
m (mass)	m_{K39}	$6.470 \cdot 10^{-26}$ kg
E (energy)	$\frac{\hbar^2}{2ma_{11}^2}$	$7.576 \cdot 10^{-27}$ J
t (time)	$\frac{2ma_{11}^2}{\hbar}$	$1.392 \cdot 10^{-8}$ s
p (momentum)	$\frac{\hbar}{a_{11}}$	$3.131 \cdot 10^{-26}$ kgm/s
k (wavenumber)	$\frac{1}{a_{11}}$	$2.969 \cdot 10^8$ m $^{-1}$
ω (frequency)	$\frac{\hbar}{2ma_{11}^2}$	$7.184 \cdot 10^7$ s $^{-1}$

4.1 Simulation parameters

After determining the unit system, we have to choose the various parameters of the simulations. For simplicity, all physical quantities will be written without mentioning of the units, throughout the text, assuming natural units. The simulation box for the non-squeezed droplet is chosen of the dimensions

$$[8000, 8000, 8000],$$

with the corresponding discretization of

$$[64, 64, 64],$$

making the discrete spacial step equal to

$$\Delta x = \frac{8000}{64} = 125.$$

The timestep is selected as $\Delta t = 50$ and the total simulation duration is

$$T_{\text{imag}} = 10^6,$$

for the imaginary time propagation, making the number of time steps

$$N_t^{(\text{imag})} = \frac{10^6}{50} = 20000.$$

Similarly, the total simulation duration for the real time propagation is

$$T_{\text{real}} = 10^7,$$

which makes the number of time steps equal to

$$N_t^{(\text{real})} = \frac{10^7}{50} = 200000.$$

Physical quantities of interest will be calculated and saved in regular time intervals, every $\Delta N_t = 100$ timesteps. All simulations will be performed across the various numbers of atoms N which can be summarized as follows

$$N \in \{100000, 250000, 500000, 750000, 1000000, 1500000, 2000000\}.$$

Last parameter of choice is the perturbation strength parameter λ , which according to the [22], has to be of order of magnitude $10^{-13} - 10^{-15}$. Therefore, all simulations were performed with

$$\lambda \in \{10^{-13}, 10^{-14}, 10^{-15}\},$$

and since for the non-squeezed droplets results did not vary at all, only results for $\lambda = 10^{-13}$ will be presented.

4.2 Results

We have propagated the excited droplet for a very long period of time, and stored $\langle Q_i(t) \rangle$ in regular time intervals. After that, we have analysed the time series by utilizing the Fourier transform. Fig. 3 (left) shows $\langle Q_0(t) \rangle$ for droplets with a selected range of atom numbers. The oscillations are clearly harmonic in nature, stable over time, and do not have any beats or complicated behaviour for larger droplets. Only the droplet with $N = 500000$ exhibits some damping over time, most likely due to unstable oscillation mode, which will be further analysed in the study of chemical potential.

The monopole strength function in logarithmic scale as a function of the excitation frequency is shown in Fig. 3 (right). The dashed vertical lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule (Eq. (3.10)), and they show great aligning with the simulation obtained peaks. This is consistent with expectations, as the main assumption in the derivation of the sum rules is that most of the mode strength has to be concentrated in a single narrow peak. The solid vertical lines represent the frequency $|\mu|/\hbar$ corresponding to the absolute value of the chemical potential $|\mu|$, obtained by the Liquid Drop Model (Eq. (3.14)). It serves a role of the atom emission threshold, the energy of oscillations required for atoms to be ejected from the droplet. We can see that the frequency of the oscillations for the $N = 500000$ droplet is slightly above the threshold, which implies that the atom emission is energetically favourable. Therefore, small droplets, excited by the $V_0 = \lambda Q_0$, have excited states which may decay by atom emission [9, 12].

The quadrupole mode is analysed in a similar way, but with a broader range of choosen values of N . Fig. 4 (left) shows $\langle Q_2(t) \rangle$ for various droplets. The oscillations are very regular and stable, across the whole range of droplets, without any signs of damping or beats. This is due to oscillation frequencies resting well bellow the stability threshold. The quadrupole strength function in logarithmic scale as a function of the excitation frequency is shown in Fig. 4 (right). Since the oscillation strength is completely concentrated in a single peak, it is expected for sum rule (Eq. (3.11)) to be an excellent estimate of the peak frequency. This has been verified by observation of the dashed vertical lines on the Fig. 4 (right).

Finally, we compare our findings with the results reported in [22] to confirm the validity of our methods and models. A direct quantitative comparison is not straightforward, as different droplet sizes were employed in the respective studies. However, a qualitative assessment reveals that both analyses yielded very similar results. This consistency strongly supports the validity of our results, especially considering that our results also exhibit excellent agreement with the analytical approximation.

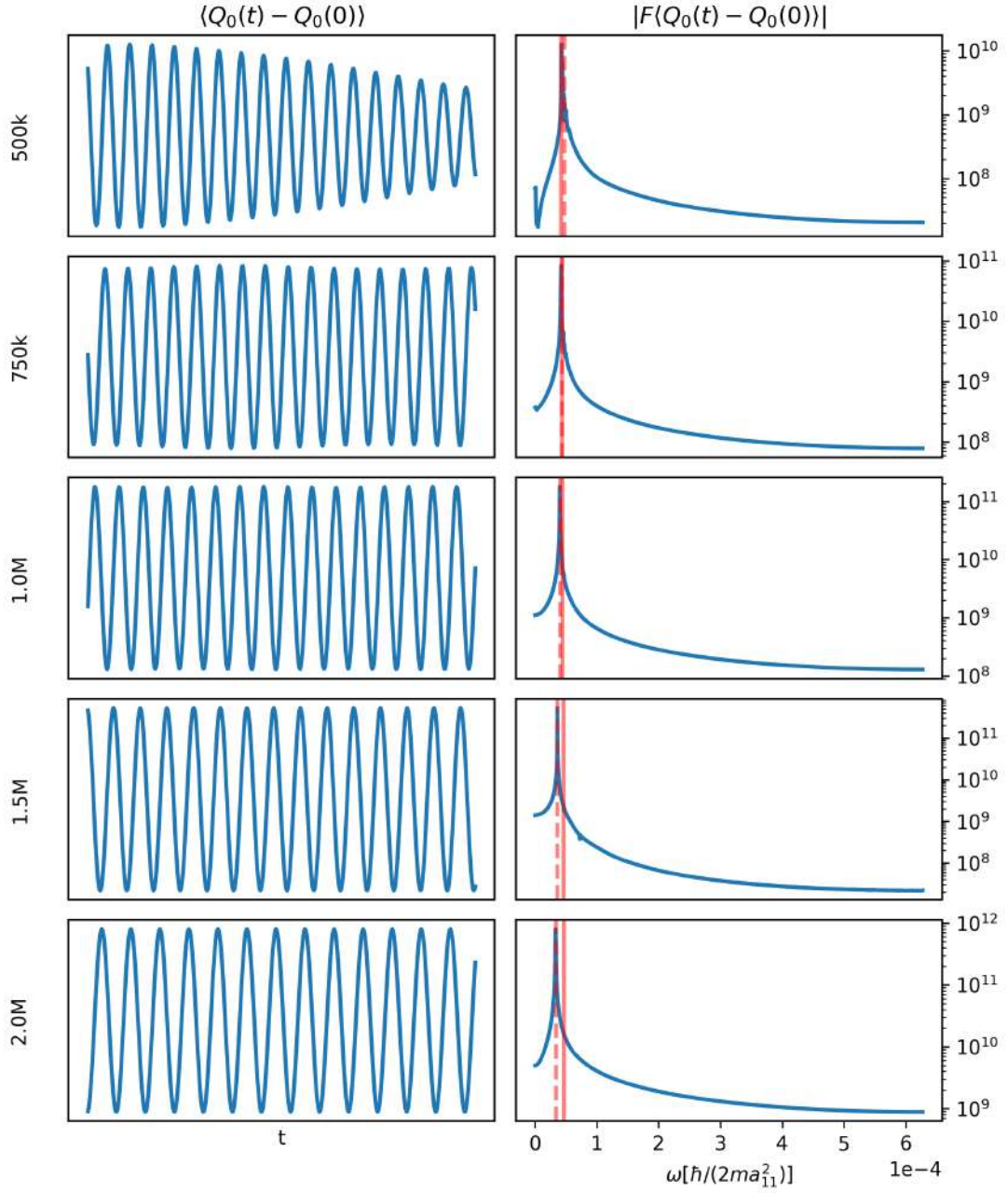


Figure 3: Time evolution of the monopole moment oscillations $\langle Q_0(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.10), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$.

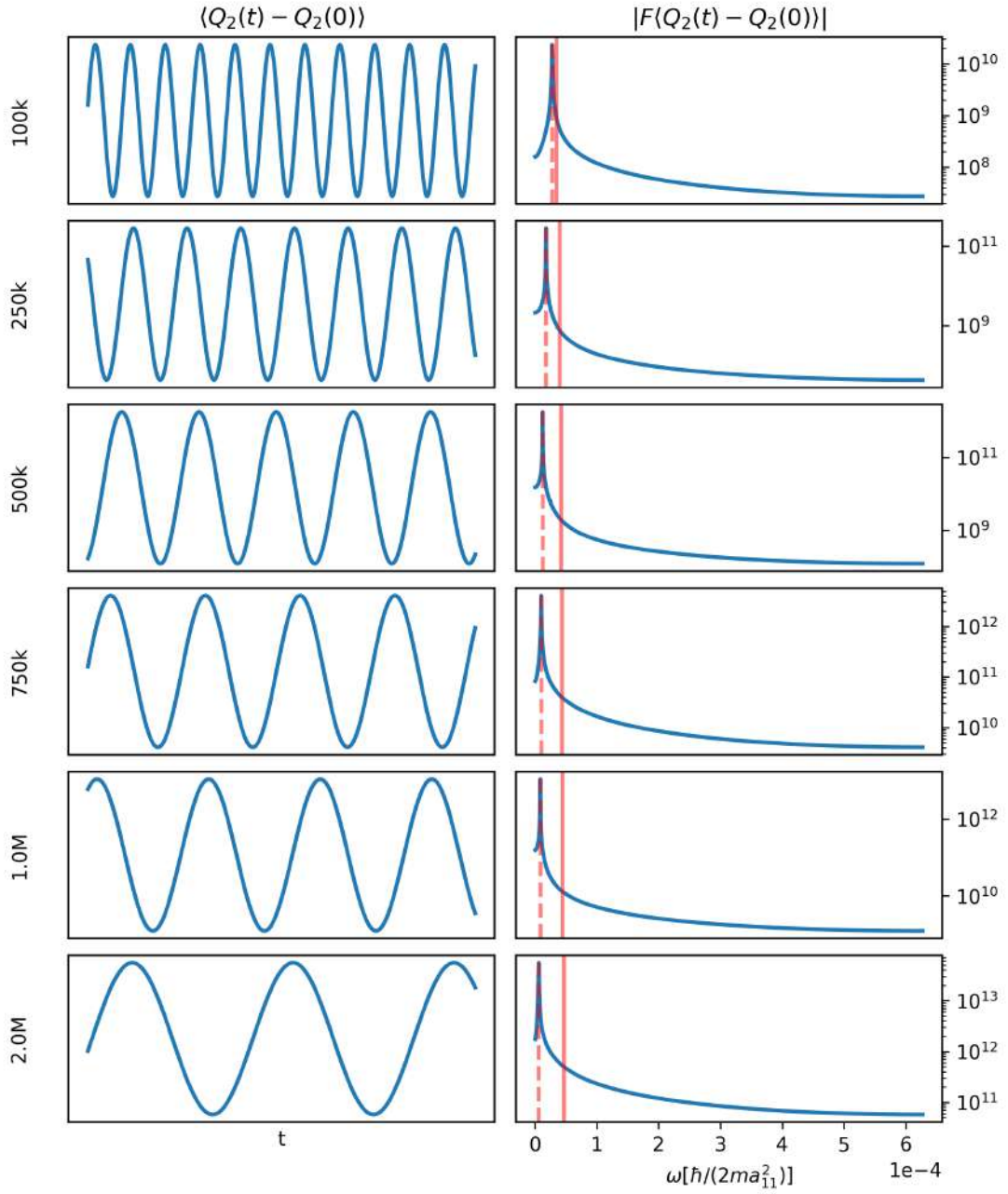


Figure 4: Time evolution of the quadrupole moment oscillations $\langle Q_2(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.11), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$.

Table 3: Liquid drop model coefficients obtained by fitting the Eq. (3.14) on results from both the QMC and MF+LHY simulations. All coefficients share the same dimension with the energy.

	E_V	E_S	E_C
QMC	$-5.31 \cdot 10^{-5}$	$1.18 \cdot 10^{-3}$	$7.44 \cdot 10^{-3}$
MF+LHY	$-4.66 \cdot 10^{-5}$	$1.02 \cdot 10^{-3}$	$6.20 \cdot 10^{-3}$

Fig. 5 shows the breathing and quadrupole frequencies, corresponding to the main peaks, as a function of the number of atoms. In this analysis, we also include the results obtained by the MF+LHY approach in order to quantify the beyond-LHY effects. We can see that the QMC functional consistently predicts higher frequencies for both the breathing and quadrupole modes, across the whole N range.

Furthermore, the chemical potential prediction based on QMC functional results is significantly higher than the one predicted by fitting on MF+LHY results. Liquid drop model coefficients for both approaches are presented in Table 3.

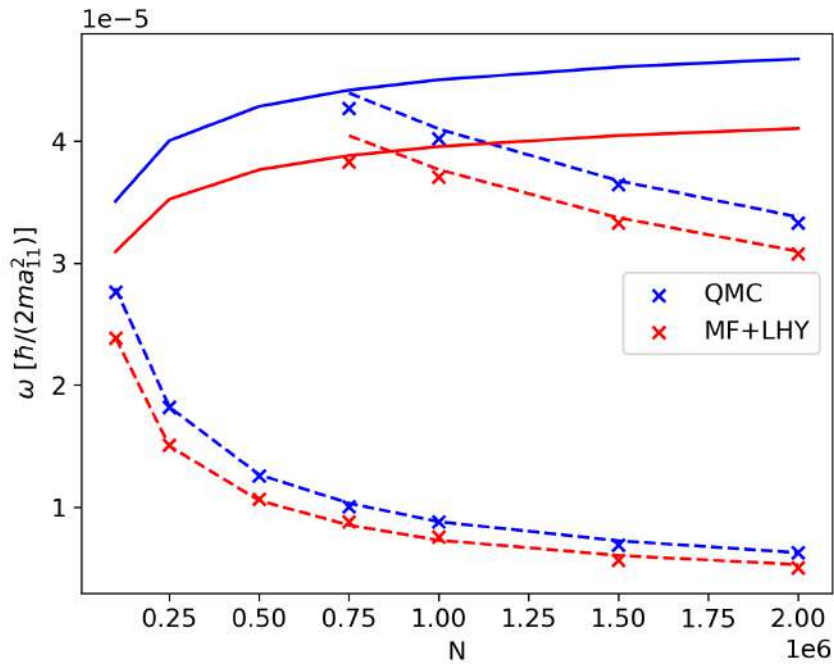


Figure 5: Breathing (upper points) and quadrupole (lower points) frequencies as a function of the number of atoms N obtained from QMC and MF+LHY simulations. Dashed lines are the $E_1/\hbar$ frequencies from the sum rules (Eq. (3.10) and (3.11)), and solid lines represent the $|\mu|/\hbar$ frequencies.

5 Study of squeezed Bose-Bose quantum droplets

In this Chapter three-dimensional squeezed Bose-Bose quantum droplets will be studied. Direction of squeezing is chosen to be the z axis. During the whole simulation procedure, strong external harmonic potential in the z axis will be added in order to squeeze the droplet, which can be written as

$$V_{\text{ho}} = \frac{m\omega^2 z^2}{2}, \quad (5.1)$$

where m is the mass of the particle and ω is the frequency of the associated harmonic oscillator. We convert it to natural units by writing

$$V_{\text{ho}} = \frac{m\omega^2 z^2}{2} = \frac{\hbar^2}{2ma_{11}^2} \cdot \frac{2ma_{11}^2}{\hbar^2} \cdot \frac{m\omega^2 z^2}{2}. \quad (5.2)$$

We recognise the first fraction as the natural unit of energy which is identically equal to one, thus we focus on rewriting the rest of the right side in a more compact form. Firstly, it has to be multiplied

$$V_{\text{ho}} = \frac{2ma_{11}^2}{\hbar^2} \cdot \frac{m\omega^2 z^2}{2} = \frac{m^2\omega^2 a_{11}^2 z^2}{\hbar^2}, \quad (5.3)$$

and since z is still in the SI units, we introduce

$$z' = \frac{z}{a_{11}}, \quad (5.4)$$

which is in the natural units. We reformulate it to $z = z'a_{11}$ and substitute into Eq. (5.3) to arrive at

$$V_{\text{ho}} = \frac{m^2\omega^2}{\hbar^2} a_{11}^4 z'^2. \quad (5.5)$$

Now, we introduce the length of the harmonic oscillator

$$a_{\text{ho}} = \sqrt{\frac{\hbar}{m\omega}}, \quad (5.6)$$

which inserted into Eq. (5.5) gives

$$V_{\text{ho}} = \frac{a_{11}^4}{a_{\text{ho}}^4} z'^2. \quad (5.7)$$

Now we can drop the prime on the z' and introduce our choice of the oscillator length

$$a_{\text{ho}} = f \cdot a_{\text{exp}}, \quad (5.8)$$

where f is an arbitrary squeezing parameter, and a_{exp} is the harmonic length of a potential used in the experiment reported in [11], which equals

$$a_{\text{exp}} = 0.639 \mu\text{m}.$$

The smaller f corresponds to a stronger confinement, while larger f leads to a less squeezed droplet. In our analysis, all simulations will be performed with

$$f \in \{0.25, 0.50, 0.75, 1.00\}, \quad (5.9)$$

and the squeezing effect on a two-dimensional cross-section density as a function of f is shown in Fig. 6.

5.1 Simulation parameters

We have to choose the wide range of parameters for the simulations. The simulation box for the droplets with $f = 1.00$ is chosen of the dimensions

$$[8000, 8000, 2000],$$

for the droplets with $f = 0.75$ it is

$$[8000, 8000, 1600],$$

while for other values of f the box is

$$[8000, 8000, 1200].$$

The corresponding number of spacial discretization steps is

$$[64, 64, 64].$$

The timestep is selected as $\Delta t = 50$ and the total simulation duration is

$$T_{\text{imag}} = 10^6,$$

for the imaginary time propagation, making the number of time steps

$$N_t^{(\text{imag})} = \frac{10^6}{50} = 20000.$$

Similarly, the total simulation duration for the real time propagation is

$$T_{\text{real}} = 10^7,$$

which makes the number of time steps equal to

$$N_t^{(\text{real})} = \frac{10^7}{50} = 200000.$$

All simulations will be performed with the extensive range of atom numbers N , which can be summarized as

$$N_{\text{BM}} \in \{25000, 50000, 75000, 100000, 200000, 300000, 400000, 500000\}$$

for the breathing mode analysis, while the range for the quadrupole mode calculations is

$$N_{\text{QM}} \in \{5000, 10000, 15000, 20000\} \cup \{N_{\text{BM}}\}.$$

Last parameter of choice is the perturbation strength parameter λ . In contrary to the non-squeezed droplets, the oscillations of the squeezed droplets show much more sensitivity to the choice of λ . Therefore, we performed simulations for the wide range of λ

$$\lambda \in \{10^{-11}, 10^{-12}, 10^{-13}, 10^{-14}, 10^{-15}\}$$

and then analysed the results in order to find the optimal value. Too strong perturbation will destroy the droplet, while too weak perturbation will not excite the desired collective oscillation modes. The results for $N = 500000$ and $f = 0.25$ are shown in Fig. 7.

We can see that the oscillations for $\lambda = 10^{-11}$ and $\lambda = 10^{-12}$, completely break down, signalling that the perturbation is too powerful. Furthermore, the oscillations for $\lambda = 10^{-14}$ and $\lambda = 10^{-15}$ have significant beating pattern, which suggests that the desired oscillation mode is not excited properly. Finally, we can conclude that the optimal value for the perturbation strength parameter is $\lambda = 10^{-13}$, which will be used throughout the remainder of this thesis.

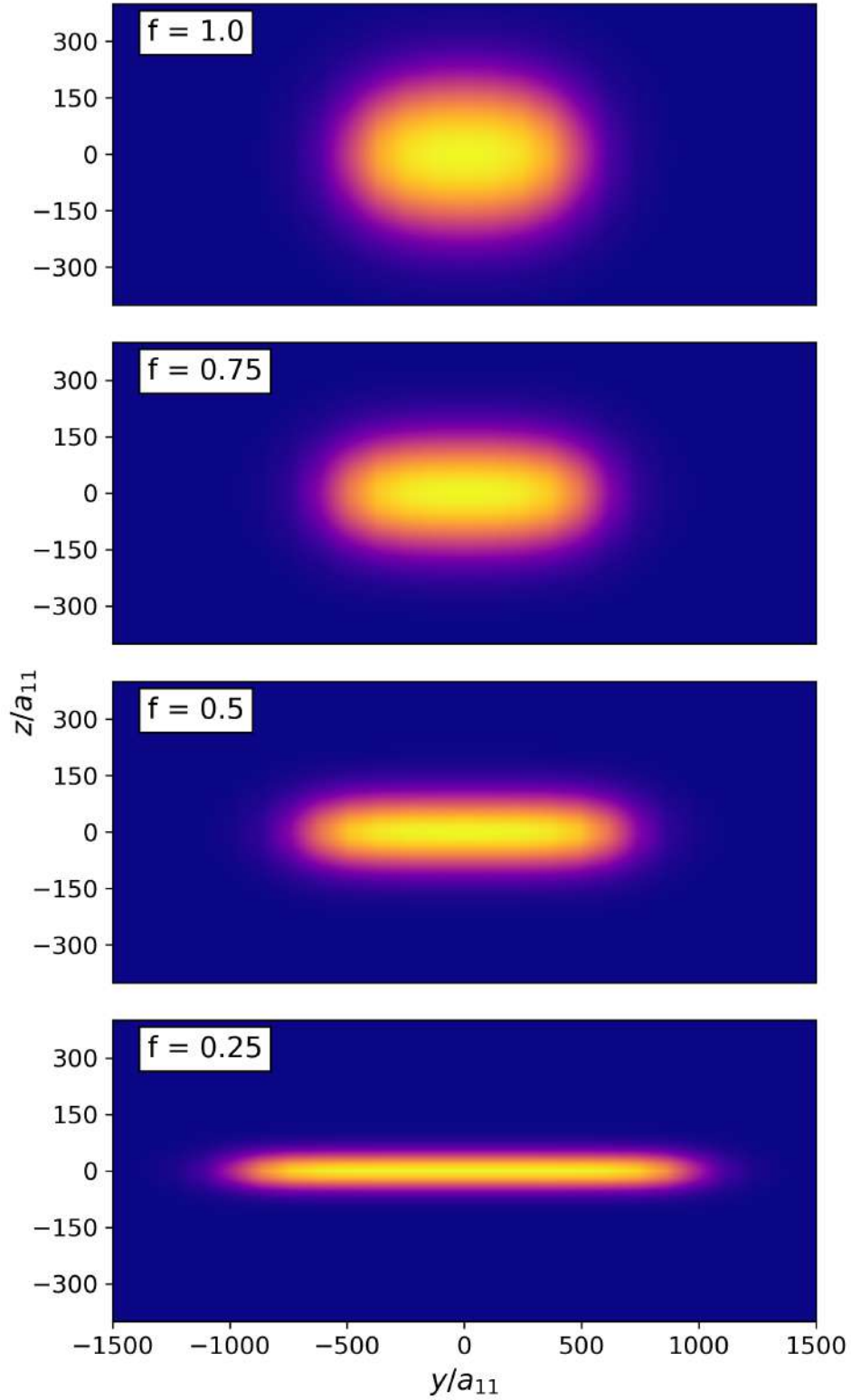


Figure 6: 2D density profiles $\rho(0, y, z)$ of droplets with 100000 atoms for the magnetic field $B = 56.230$ G and different squeezing strengths, described by the harmonic oscillator length of $a_{ho} = f \times 0.639 \mu\text{m}$. Beware of the different scales on the y axis (perpendicular to squeezing) and on the z axis which is in the direction of the squeezing.

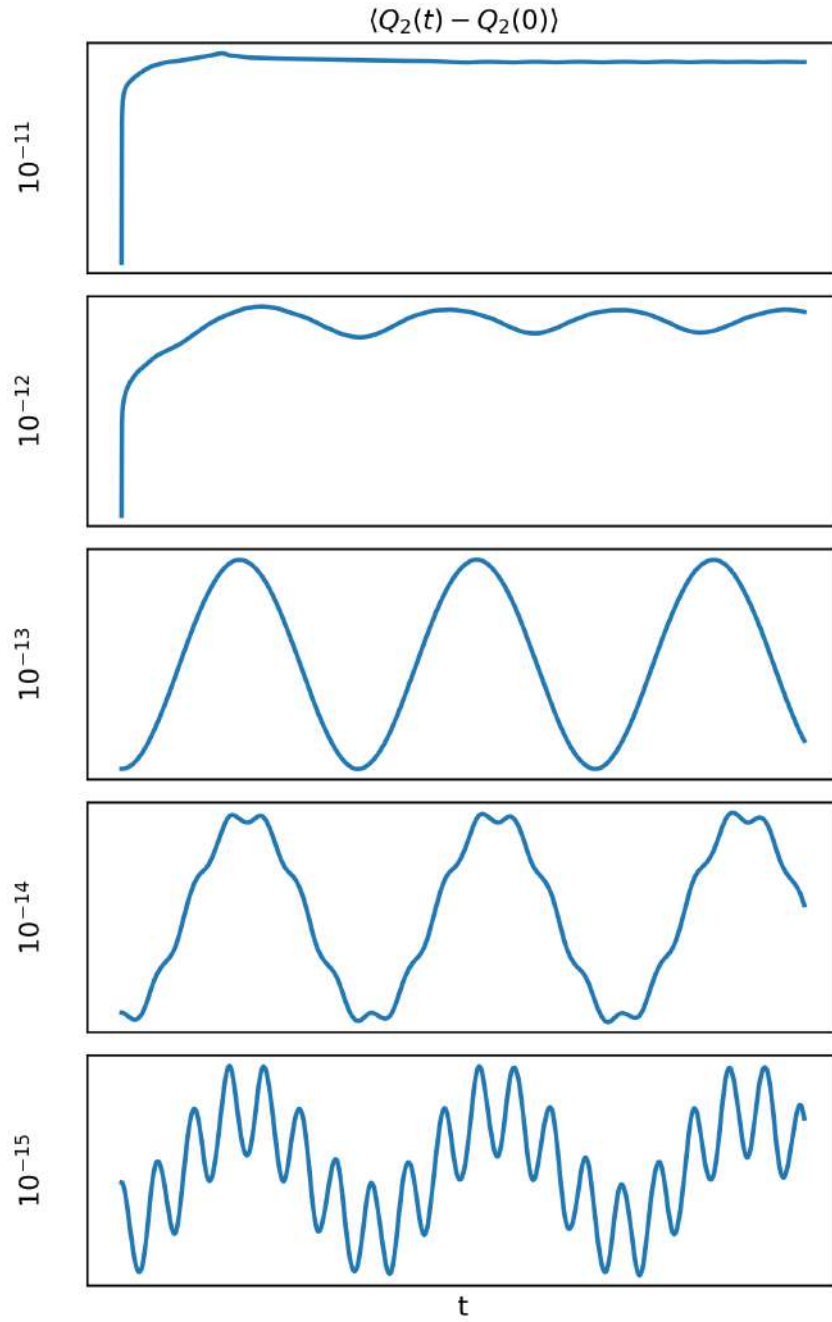


Figure 7: Time evolution of the quadrupole moment oscillations $\langle Q_2(t) \rangle$, obtained by the QMC energy functional, across the range of λ values, which are shown on the left side. The droplet has $N = 500000$ atoms, and the squeezing parameter is $f = 0.25$.

5.2 Breathing mode

We have propagated the excited droplet for a very long period of time, and stored $\langle Q_0(t) \rangle$ in regular time intervals. After that, the stored time series has been analysed by applying the Fourier transform. Fig. 8 (left) shows $\langle Q_0(t) \rangle$ for various droplets squeezed by the squeezing parameter $f = 0.25$. Also, Fig. 9 (left) presents the oscillations for droplets confined by $f = 1.00$. Plots for two other confinement strengths can be found in the Appendix A.

Figs. 8 (right) and 9 (right) show the monopole strength function in logarithmic scale as a function of the excitation frequency. The dashed vertical lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule (3.10), and they show exceptional agreement with the peaks obtained by simulations. This aligns with the expectations, as the main assumption of the sum rules is that most of the oscillation mode energy has to be concentrated in a single narrow peak. For all values of f , we can see a dominant peak only accompanied by a strange peak of lesser strength in the higher frequency range. One significant property we can notice is that for the same value of f , its frequency seems constant in value. This could be in relation to the frequency of the squeezing potential, but further analysis is required to eliminate the possibility of numerical artefacts.

For $f = 0.25$, oscillations are clearly harmonic and stable for droplets with $N = 50000$ or more atoms. Only the droplet with $N = 25000$ exhibits beating behaviour which can be explained as the peak frequency predicted by the sum rules crossed over the stability threshold. On the other side of the spectrum, for $f = 1.00$, this behaviour is extended to the $N = 50000$ and $N = 75000$ droplets, only $N = 100000$ being stable and harmonic. It also can be explained by the relation between predicted oscillation frequency and the $|\mu|/\hbar$ as the stability threshold.

The Liquid Drop Model (Eq. (3.14)) has been employed for the calculation of the chemical potential. It is shown on Figs. 8 (right) and 9 (right) as the vertical solid line. It serves a purpose as the atom emission threshold, the oscillation energy required for atoms to be ejected from the droplet. As mentioned earlier, we can see that smaller droplets tend to have excited states that can decay by atom emission. Stronger confinement drives that limit down, which makes sense as the droplets need lesser atom numbers in order to possess similar properties.

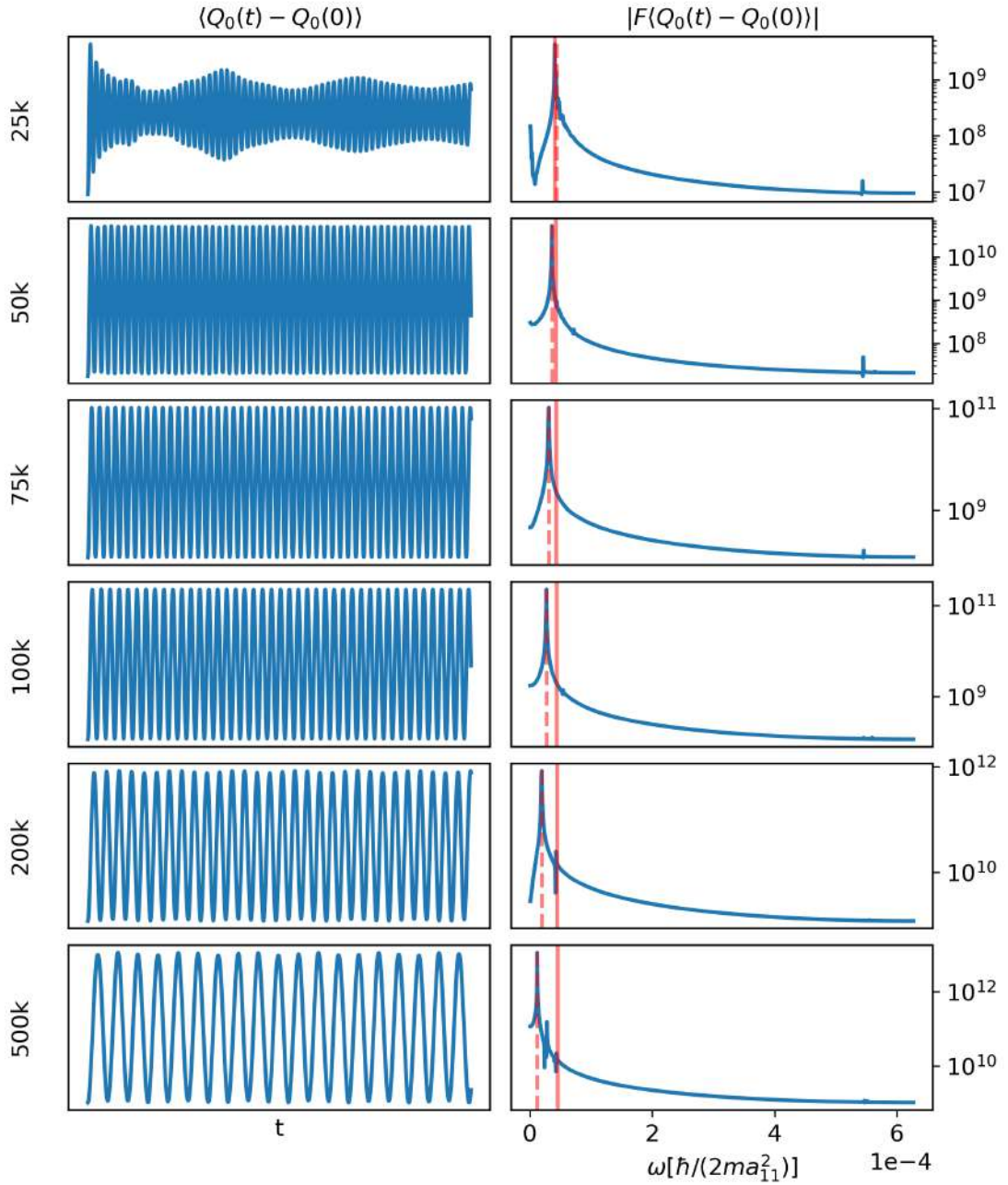


Figure 8: Time evolution of the monopole moment oscillations $\langle Q_0(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.10), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 0.25$.

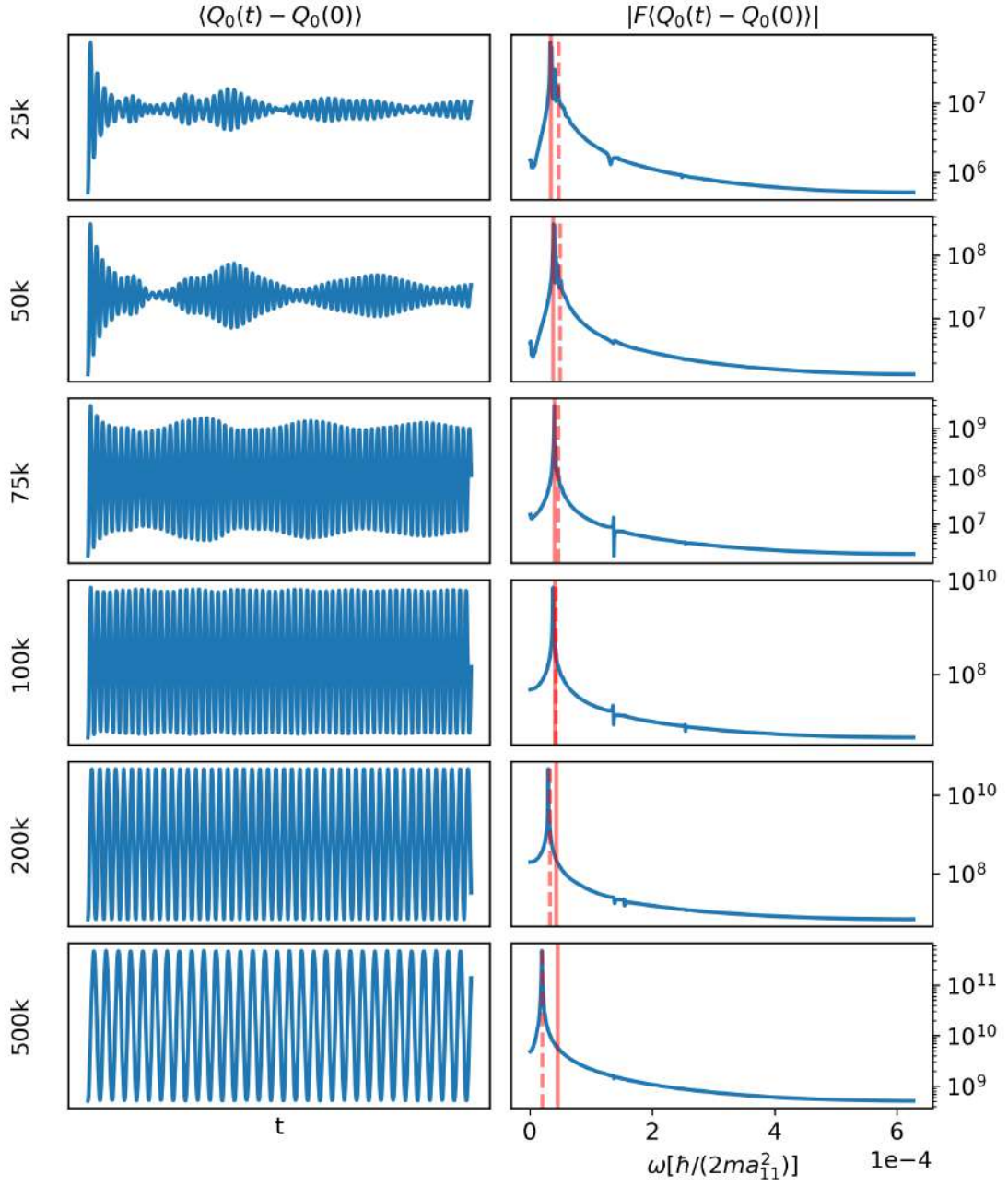


Figure 9: Time evolution of the monopole moment oscillations $\langle Q_0(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.10), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 1.00$.

5.3 Quadrupole mode

The excited droplet was propagated for a very long period of time in a real time propagation, and $\langle Q_2(t) \rangle$ was stored in regular time intervals. Secondly, the time series was analysed by utilizing the Fourier transform to obtain the frequency spectrum. Fig. 10 (left) shows $\langle Q_2(t) \rangle$ across the selected array of droplet sizes, squeezed by the squeezing parameter $f = 0.25$. For the droplets with $f = 1.00$ squeezing, the oscillations are presented on Fig. 11 (left). Plots for $f = 0.50$ and $f = 0.75$ are located in the Appendix A.

Figs. 10 (right) and 11 (right) show the quadrupole strength function in logarithmic scale as a function of the excitation frequency. The dashed vertical lines represent the frequency $E_1/\hbar$ obtained by the sum rule (3.11), and they shown extraordinary alignment with the peaks calculated from the simulations. This is in line with the expectations, as the core assumption for sum rules to hold, is that the majority of the oscillation mode energy is concentrated in a single narrow peak. It even gives excellent results for the droplets that have a second significant peak, showing universality of this approach for the peak frequency approximation. For some droplets we can notice the small peak at the very high frequency, similar to one observed in the monopole analysis. It also seems as the frequencies of that peaks align between all simulations with the same f , further warranting our assumption of it being directly related to the frequency of the harmonic squeezing potential.

For the smallest f , oscillations seem to be stable and mostly harmonic, but we can notice the second peak showing at higher frequency, just under the stability threshold. Larger droplets seem to have a single peak frequency, which dominates other possible peaks. As an example, the oscillation energy for the droplet with $N = 500000$ is completely concentrated in a single narrow peak. The droplets with the least confinement show great stability of their oscillations, and the frequency spectrum is dominated by a single peak. Only the small droplet with $N = 25000$ exhibits damped oscillations with the traces of beats. This is clearly the result of peak frequency exceeding the stability threshold.

The chemical potential μ was calculated using the LDM (3.14). It is shown on Figs. 10 (right) and 11 (right) as the vertical solid line. The accompanied frequency $|\mu|/\hbar$ has a role of the stability threshold, the oscillation energy needed for atoms to be ejected from the droplet. The quadrupole oscillations tend to be more stable across the whole range of f and N , only the $N = 25000$ atom droplet becoming unstable for the squeezing strength $f = 1.00$. We can conclude that the strongly confined droplets can exhibit stable quadrupole collective oscillations for very small atom numbers.

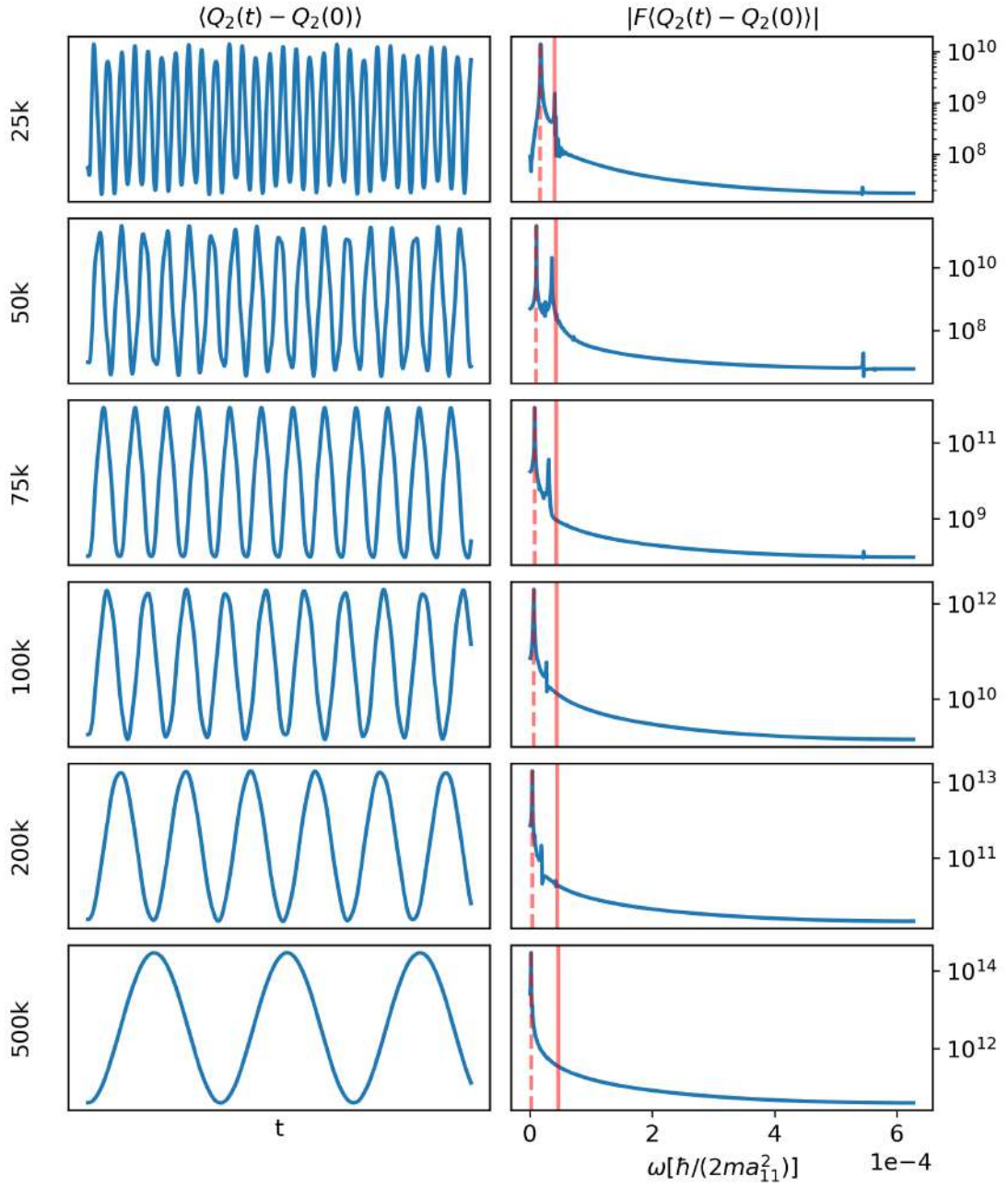


Figure 10: Time evolution of the quadrupole moment oscillations $\langle Q_2(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.11), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 0.25$.

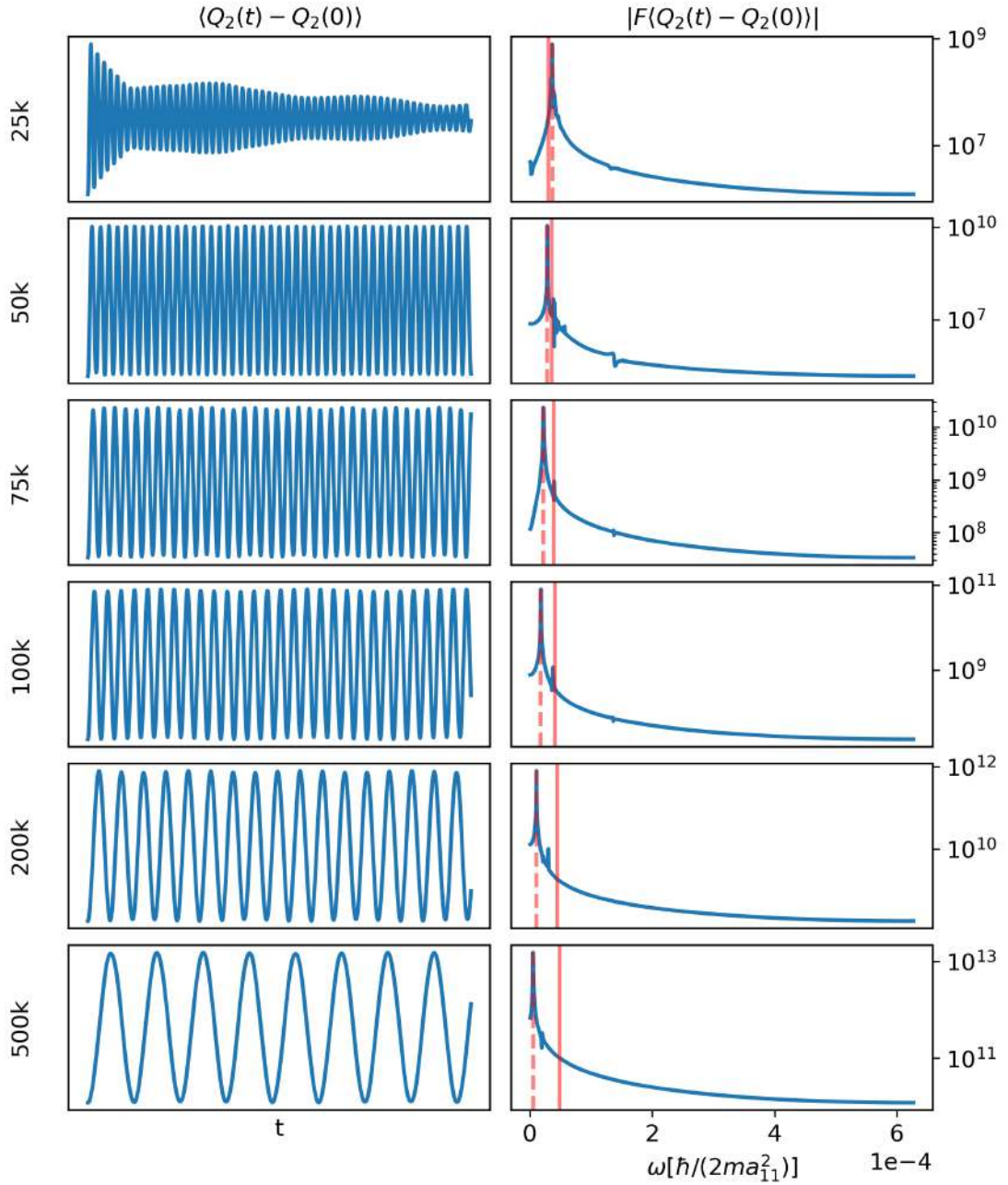


Figure 11: Time evolution of the quadrupole moment oscillations $\langle Q_2(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.11), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 1.00$.

5.4 Comparison with MF+LHY approach

We show in Figs. 12 - 15 the breathing and quadrupole peak frequencies, as a function of the number of atoms obtained with the QMC functional and the MF+LHY approach. As we can see, the QMC functional approach gives systematically higher values for the peak frequencies, across the whole N range. This gap is significantly more pronounced for the breathing mode calculations, especially for higher f values. For the $f = 0.25$ squeezing, quadrupole mode calculations give very similar results for both approaches. One possible explanation is that beyond-LHY effects are greater in the three-dimensional droplet, since stronger squeezing approaches quasi-two-dimensional regime.

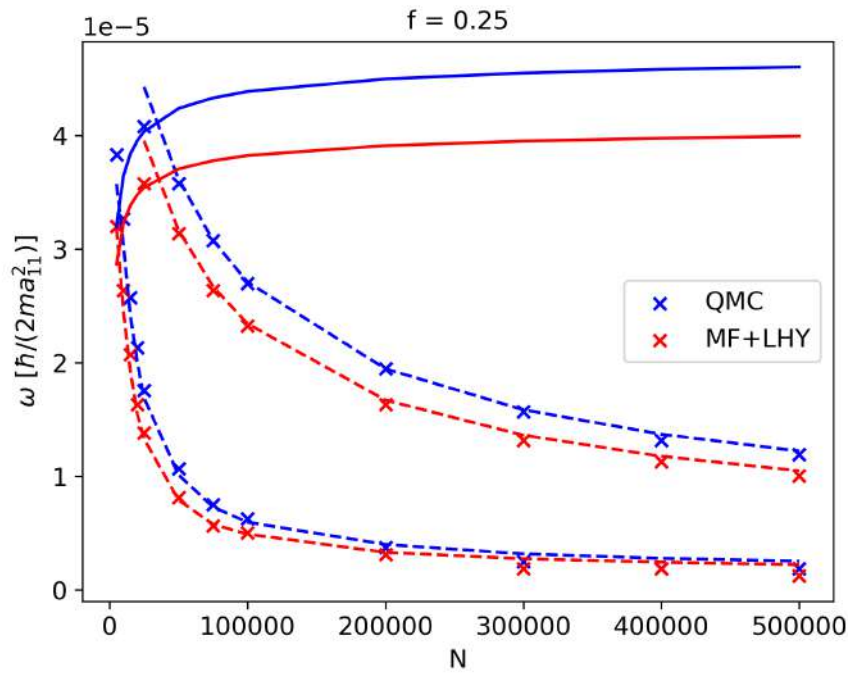


Figure 12: Breathing (upper points) and quadrupole (lower points) frequencies as a function of the number of atoms N obtained from QMC and MF+LHY simulations. Dashed lines are the $E_1/\hbar$ frequencies from the sum rules (Eq. (3.10) and (3.11)), and solid lines represent the $|\mu|/\hbar$ frequencies. The squeezing parameter is $f = 0.25$.

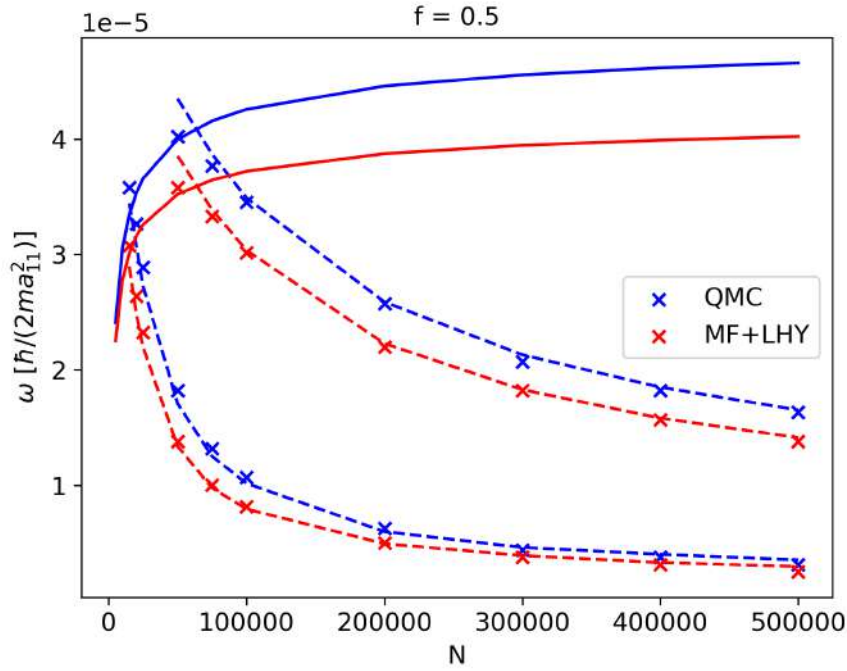


Figure 13: Breathing (upper points) and quadrupole (lower points) frequencies as a function of the number of atoms N obtained from QMC and MF+LHY simulations. Dashed lines are the $E_1/\hbar$ frequencies from the sum rules (Eq. (3.10) and (3.11)), and solid lines represent the $|\mu|/\hbar$ frequencies. The squeezing parameter is $f = 0.50$.

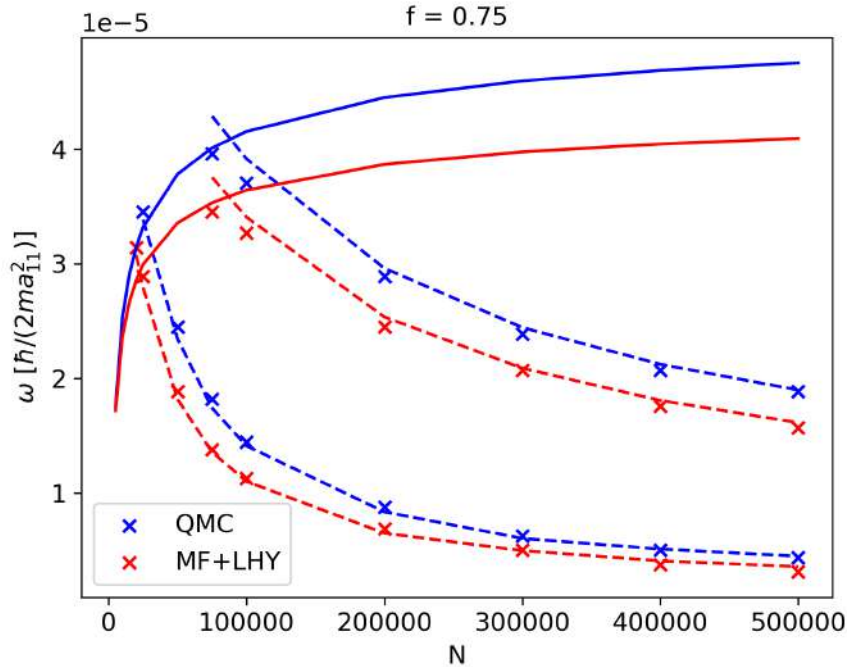


Figure 14: Breathing (upper points) and quadrupole (lower points) frequencies as a function of the number of atoms N obtained from QMC and MF+LHY simulations. Dashed lines are the $E_1/\hbar$ frequencies from the sum rules (Eq. (3.10) and (3.11)), and solid lines represent the $|\mu|/\hbar$ frequencies. The squeezing parameter is $f = 0.75$.

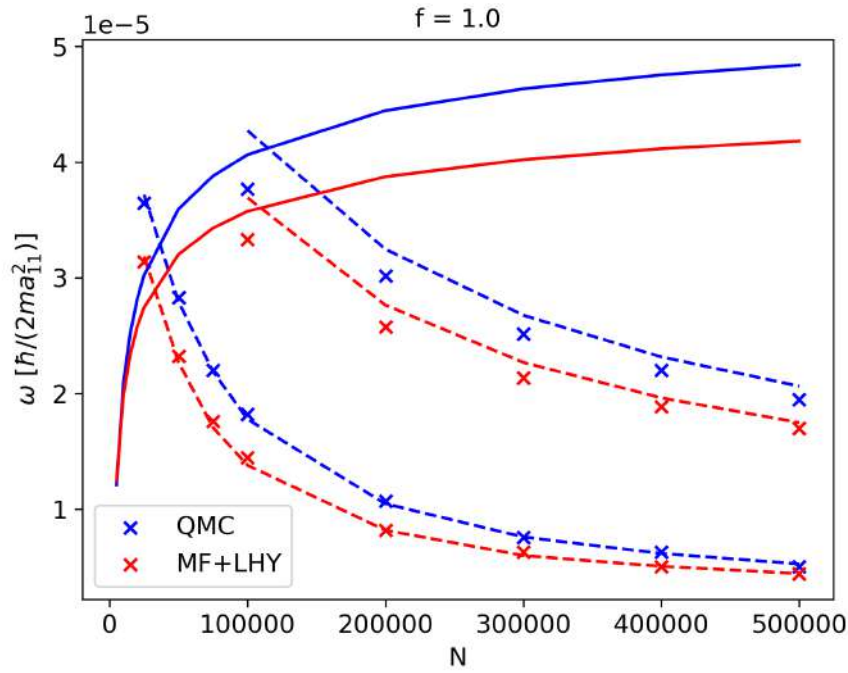


Figure 15: Breathing (upper points) and quadrupole (lower points) frequencies as a function of the number of atoms N obtained from QMC and MF+LHY simulations. Dashed lines are the $E_1/\hbar$ frequencies from the sum rules (Eq. (3.10) and (3.11)), and solid lines represent the $|\mu|/\hbar$ frequencies. The squeezing parameter is $f = 1.00$.

Table 4: Liquid drop model coefficients obtained by fitting the Eq. (3.14) on results from both the QMC and MF+LHY simulations, for different values of the squeezing strength parameter f . All coefficients share the same dimension with the energy.

f	Functional	$E_V [10^{-5}]$	$E_S [10^{-4}]$	$E_C [10^{-3}]$
0.25	QMC	-4.860	2.726	5.235
	MF+LHY	-4.190	2.057	4.571
0.50	QMC	-5.194	6.176	3.305
	MF+LHY	-4.408	4.360	4.020
0.75	QMC	-5.601	10.213	-1.142
	MF+LHY	-4.717	7.371	1.090
1.00	QMC	-5.989	14.073	-6.182
	MF+LHY	-5.066	10.735	-3.203

5.5 Comparison between squeezing strengths

Now, we will briefly discuss effects of different squeezing strengths on the peak frequencies of both breathing and quadrupole modes. Fig. 16 shows the breathing mode peak frequency as the function of the number of atoms N for different squeezing parameters f , and the Fig. 17 shows the same for the quadrupole mode. For both modes, we can see that the stronger squeezing lowers the peak frequency across the whole N range. It can be noted that the sum rule approach works much better for the quadrupole mode for every f , especially for the lower N range. Also, we notice that the frequencies for the breathing mode at $f = 1.00$ deviate significantly from the sum rule approach.

It is also interesting to investigate how LDM coefficients depend on the value of f , since every coefficient has a direct physical interpretation. First, let's recall the energy per particle derived from the liquid drop model

$$\frac{E}{N} = E_V + E_S x + E_C x^2 \quad (5.10)$$

where $x = N^{-1/3}$. The first term is known as the volume term, second term corresponds to the surface energy, and the third term is called the curvature energy. Corresponding coefficients are E_V , E_S and E_C , respectively, and they are showed in the Table 4 for both the QMC and the MF+LHY approach, across different f values.

As we can see, the coefficients from QMC simulations tend to have greater absolute value than the MF+LHY counterparts, keeping the same sign. All E_V values are negative, all E_S values are positive and the most of the E_C values are positive. With increasing confinement strength, energy from the curvature rises due to sharper curves on the edge of the squeezed droplets as opposed to the spherical droplets. Also, the volume energy increases, while the surface term decreases.

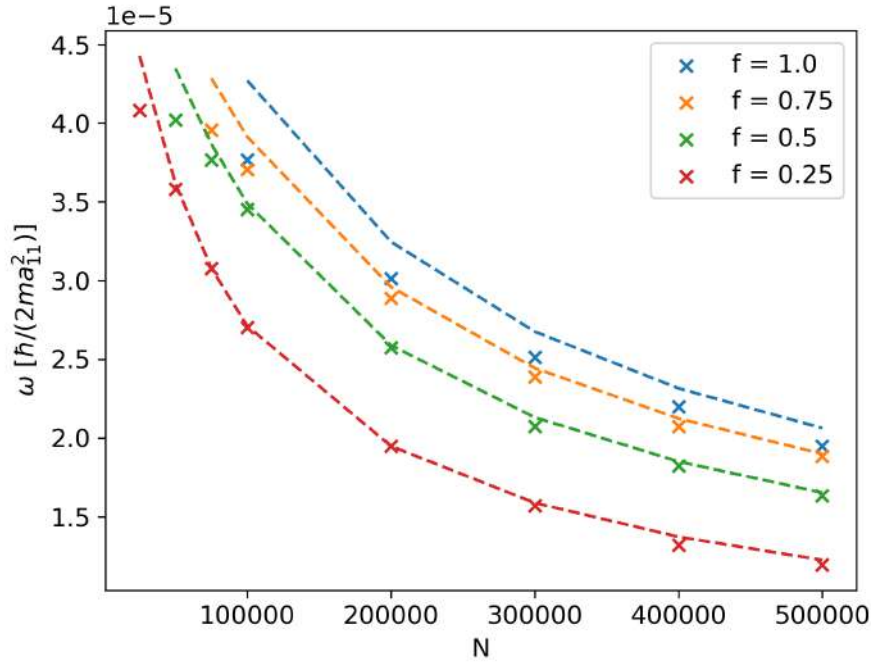


Figure 16: Breathing mode frequencies as a function of the number of atoms N compared between various squeezing strength parameters f , obtained by the QMC functional simulations. Dashed lines correspond to the $E_1/\hbar$ frequencies from the sum rule (Eq. (3.10)).

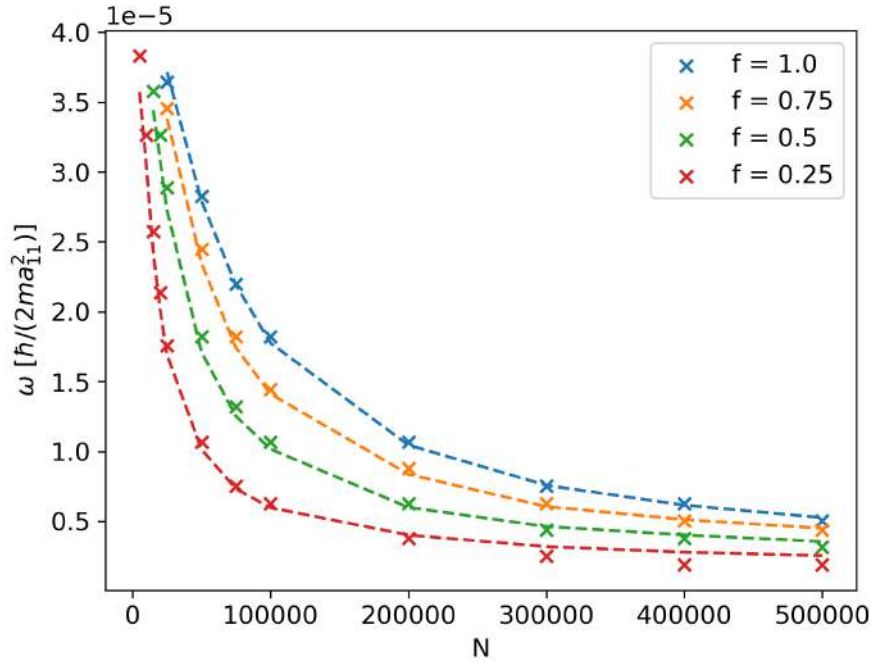


Figure 17: Quadrupole mode frequencies as a function of the number of atoms N compared between various squeezing strength parameters f , obtained by the QMC functional simulations. Dashed lines correspond to the $E_1/\hbar$ frequencies from the sum rule (Eq. (3.11)).

6 Conclusion

In this thesis, we studied the collective oscillations in squeezed self-bound Bose-Bose droplets, as a function of droplet size and confinement strength. To achieve this, we employed a robust numerical approach based on Density Functional Theory, using an energy functional derived from exact Quantum Monte Carlo data. The validity of our simulation procedure was first established in the non-squeezed case, where our results showed excellent agreement with previous work on the topic [22]. This provided a strong foundation for the central investigation of squeezed droplets. Our primary finding is that increasing confinement strength significantly lowers the frequencies of both the monopole and quadrupole modes. This behaviour was accurately captured by an analytical sum-rule approach, affirming its role as a practical tool for quickly predicting peak frequencies. Also, by introducing a Liquid Drop Model to connect the chemical potential to the number of atoms, we established a clear stability threshold. This model proved to be exceptionally powerful, successfully explaining every observed instance of mode damping or deviation.

The implications of these findings are significant for future research. First, the discovery that squeezing lowers the critical number of atoms required for a droplet to be self-bound suggests that squeezed droplets are more experimentally accessible than spherical droplets. This could lower the technical barrier for creating and studying these systems. Second, the significant frequency shifts provide clear, testable signatures for experimentalists to probe the dimensional crossover and the nature of beyond-mean-field effects.

This study was conducted under the assumption of zero temperature, therefore its limitation is the neglect of thermal fluctuations, which could introduce additional oscillation damping and shift the frequencies in a real experimental setup. Furthermore, our model does not account for inelastic three-body loss processes, which may become relevant to the lifetime of strongly squeezed droplets. It would also be useful to extend the study to other values of experimentally accessible magnetic fields.

This work opens several exciting avenues for future research. An immediate theoretical extension would be to incorporate finite-temperature effects into the simulations to provide an even more direct comparison with experiments. Furthermore, applying this validated methodology to explore other geometries, or to investigate the dynamics of droplets in Bose-Fermi mixtures, would provide deeper insights into the fascinating world of self-bound quantum systems.

7 Bibliography

- [1] A. Einstein: *Quantum theory of the monoatomic ideal gas*, Part I and Part II, Sitzungsber. Preuss. Akad. Wiss., 1:3-14, 1925.
- [2] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman and E. A. Cornell: *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor*, Science, 269(5221), 198-201, 1995.
DOI: <https://doi.org/10.1126/science.269.5221.198>
- [3] K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn and W. Ketterle: *Bose-Einstein Condensation in a Gas of Sodium Atoms*: Phys. Rev. Lett., 75, 3969, 1995.
DOI: <https://doi.org/10.1103/PhysRevLett.75.3969>
- [4] C. Chin, R. Grimm, P. Julienne and E. Tiesinga: *Feshbach resonances in ultracold gases*, Rev. Mod. Phys., 82, 1225, 2010.
DOI: <https://doi.org/10.1103/RevModPhys.82.1225>
- [5] E. P. Gross: *Structure of a quantized vortex in boson systems*, Nuovo Cim 20, 454-477, 1961.
DOI: <https://doi.org/10.1007/BF02731494>
- [6] L. Pitaevskii: *Vortex Lines in an Imperfect Bose Gas*, Journal of Experimental and Theoretical Physics, 13, 451-454, 1961.
- [7] T. Lee and C. Yang: *Many-body problem in quantum mechanics and quantum statistical mechanics*, Physical Review, vol. 105, no. 3, p. 1119, 1957.
DOI: <https://doi.org/10.1103/PhysRev.105.1119>
- [8] K. Huang and C. N. Yang: *Quantum-mechanical many-body problem with hard-sphere interaction*, Physical Review, vol. 105, no. 3, p. 767, 1957.
DOI: <https://doi.org/10.1103/PhysRev.105.767>
- [9] D. Petrov: *Quantum mechanical stabilization of a collapsing Bose-Bose mixture*, Phys. Rev. Lett., vol. 115, no. 15, p. 155302, 2015.
DOI: <https://doi.org/10.1103/PhysRevLett.115.155302>
- [10] I. F. Barbut, H. Kadau, M. Schmitt, M. Wenzel and T. Pfau: *Observation of quantum droplets in a strongly dipolar Bose gas*, Phys. Rev. Lett., vol. 116, 215301, 2016.
DOI: <https://doi.org/10.1103/PhysRevLett.116.215301>
- [11] C. Cabrera, L. Tanzi, J. Sanz, B. Naylor, P. Thomas, P. Cheiney and L. Tarruell: *Quantum liquid droplets in a mixture of Bose-Einstein condensates*, Science 359, 301, 2018.

DOI: <https://doi.org/10.1126/science.aao5686>

- [12] G. Ferioli, G. Semeghini, S. Terradas-Briansó, L. Masi, M. Fattori and M. Modugno: *Dynamical formation of quantum droplets in a 39K mixture*, Phys. Rev. Research, vol. 2, no. 1, p. 013269, 2020.
DOI: <https://doi.org/10.1103/PhysRevResearch.2.013269>
- [13] V. Cikojević, L. Vranješ Markić, M. Pi, M. Barranco and J. Boronat: *Towards a quantum Monte Carlo-based density functional including finite-range effects: Excitation modes of a 39K quantum droplet*, Phys. Rev. A, 102, 033335, 2020.
DOI: <https://doi.org/10.1103/PhysRevA.102.033335>
- [14] H. Hu and X.-J. Liu: *Collective oscillations of a spherical ultradilute quantum droplet*, Phys. Rev. A, 102, 053303, 2020.
DOI: <https://doi.org/10.1103/PhysRevA.102.053303>
- [15] P. Zin, M. Pylak, T. Wasak, M. Gajda and Z. Idziaszek: *Quantum Bose-Bose droplets at a dimensional crossover*, Phys. Rev. A, 98, 051603, 2018.
DOI: <https://doi.org/10.1103/PhysRevA.98.051603>
- [16] T. Ilg, J. Kumlin, L. Santos, D. Petrov and H. P. Büchler: *Dimensional crossover for the beyond-mean-field correction in Bose gases*, Phys. Rev. A, 98, 051604(R), 2018.
DOI: <https://doi.org/10.1103/PhysRevA.98.051604>
- [17] P. Cheiney, C. R. Cabrera, J. Sanz, B. Naylor, L. Tanzi and L. Tarruell: *Bright Soliton to Quantum Droplet Transition in a Mixture of Bose-Einstein Condensates*, Phys. Rev. Lett., 120, 135301, 2018.
DOI: <https://doi.org/10.1103/PhysRevLett.120.135301>
- [18] A. Sanuy, R. Barač, P. Stipanović, L. Vranješ Markić and J. Boronat: *Squeezing Bose-Bose liquid drops*, Physical Review A, vol. 109, no. 1, 013313, 2024.
DOI: <https://doi.org/10.1103/PhysRevA.109.013313>
- [19] V. Cikojević, L. Vranješ Markić and J. Boronat: *Finite-range effects in ultradilute quantum drops*, New J. Phys., 22, 053045, 2020.
DOI: <https://doi.org/10.1088/1367-2630/ab867a>
- [20] Lev Pitaevskii and Sandro Stringari: *Bose-Einstein Condensation and superfluidity*, Oxford University Press, Oxford, 2016.
- [21] C. J. Petchick and H. Smith: *Bose-Einstein Condensation in Dilute Gases*, 2nd Edition, Cambridge University Press, Cambridge, 2008.

- [22] Viktor Cikojević: *Ab-initio Quantum Monte Carlo study of ultracold atomic mixtures*, Doctoral thesis, University of Zagreb and Universitat Politecnica de Catalunya, 2021.
DOI: <https://doi.org/10.48550/arXiv.2105.01439>
- [23] H. T. Stoof, K. B. Gubbels and D. B. Dickerscheid: *Ultracold quantum fields*, Springer, 2009.
- [24] E. M. Lifshitz and L. P. Pitaevskii: *Statistical physics: theory of the condensed state (part 2)*, vol. 9, Elsevier, 2013.
- [25] N. Bogoliubov: *On the theory of superfluidity*, J. Phys, vol. 11, no. 1, p. 23, 1947.
- [26] E. Braaten, H. W. Hammer and S. Hermans: *Nonuniversal effects in the homogeneous Bose gas*, Phys. Rev. A, vol. 63, no. 6, p. 063609, 2001.
DOI: <https://doi.org/10.1103/PhysRevA.63.063609>
- [27] S. Giorgini, J. Boronat and J. Casulleras: *Ground state of a homogeneous Bose gas: A diffusion Monte Carlo calculation*, Phys. Rev. A, vol. 60, no. 6, p. 5129, 1999.
DOI: <https://doi.org/10.1103/PhysRevA.60.5129>
- [28] E. Braaten and A. Nieto: *Quantum corrections to the ground state of a trapped Bose-Einstein condensate*, Phys. Rev. B, vol. 56, no. 22, p. 14745, 1997.
DOI: <https://doi.org/10.1103/PhysRevB.56.14745>
- [29] D. Blume and C. H. Greene, *Quantum corrections to the ground-state energy of a trapped Bose-Einstein condensate: A diffusion Monte Carlo calculation*, Phys. Rev. A, vol. 63, no. 6, p. 063601, 2001.
DOI: <https://doi.org/10.1103/PhysRevA.63.063601>
- [30] P. Hohenberg and W. Kohn, *Inhomogeneous electron gas*, Physical Review, vol. 136, no. 3B, p. B864, 1964.
DOI: <https://doi.org/10.1103/PhysRev.136.B864>
- [31] E. Eberhard and R. Dreizler, *Density Functional Theory: An Advanced Course*, Springer, Berlin, 2011.
- [32] D. Petrov and G. E. Astrakharchik: *Ultradilute Low-Dimensional Liquids*, Phys. Rev. Lett., 117, 100401, 2016.
DOI: <https://doi.org/10.1103/PhysRevLett.117.100401>
- [33] D. M. Larsen: *Binary mixtures of dilute bose gases with repulsive interactions at low temperature*, Annals of Physics, New York, vol. 24, p. 89-101, 1963.
DOI: [https://doi.org/10.1016/0003-4916\(63\)90066-6](https://doi.org/10.1016/0003-4916(63)90066-6)

- [34] F. Ancilotto, M. Barranco, M. Guilleumas and M. Pi: *Self-bound ultradilute Bose mixtures within local density approximation*, Phys. Rev. A, vol. 98, no. 5, p. 053623, 2018.
DOI: <https://doi.org/10.1103/PhysRevA.98.053623>
- [35] F. Minardi, F. Ancilotto, A. Burchianti, C. D’Errico, C. Fort and M. Mondugno: *Effective expression of the Lee-Huang-Yang energy functional for heteronuclear mixtures*, Phys. Rev. A, vol. 100, no. 6, p. 063636, 2019.
DOI: <https://doi.org/10.1103/PhysRevA.100.063636>
- [36] O. Bohigas, A. M. Lane and J. Martorell: *Sum rules for nuclear collective excitations*, Physics Reports, vol. 51, no. 5, p. 267-316, 1979.
DOI: [https://doi.org/10.1016/0370-1573\(79\)90079-6](https://doi.org/10.1016/0370-1573(79)90079-6)
- [37] O. Falou: *Modelling high frequency ultrasound scattering from cells and ultrasound contrast agents*, Doctoral thesis, Ryerson University, Toronto, Canada, 2011.
DOI: <https://doi.org/10.32920/ryerson.14658069.v1>

A Graphs

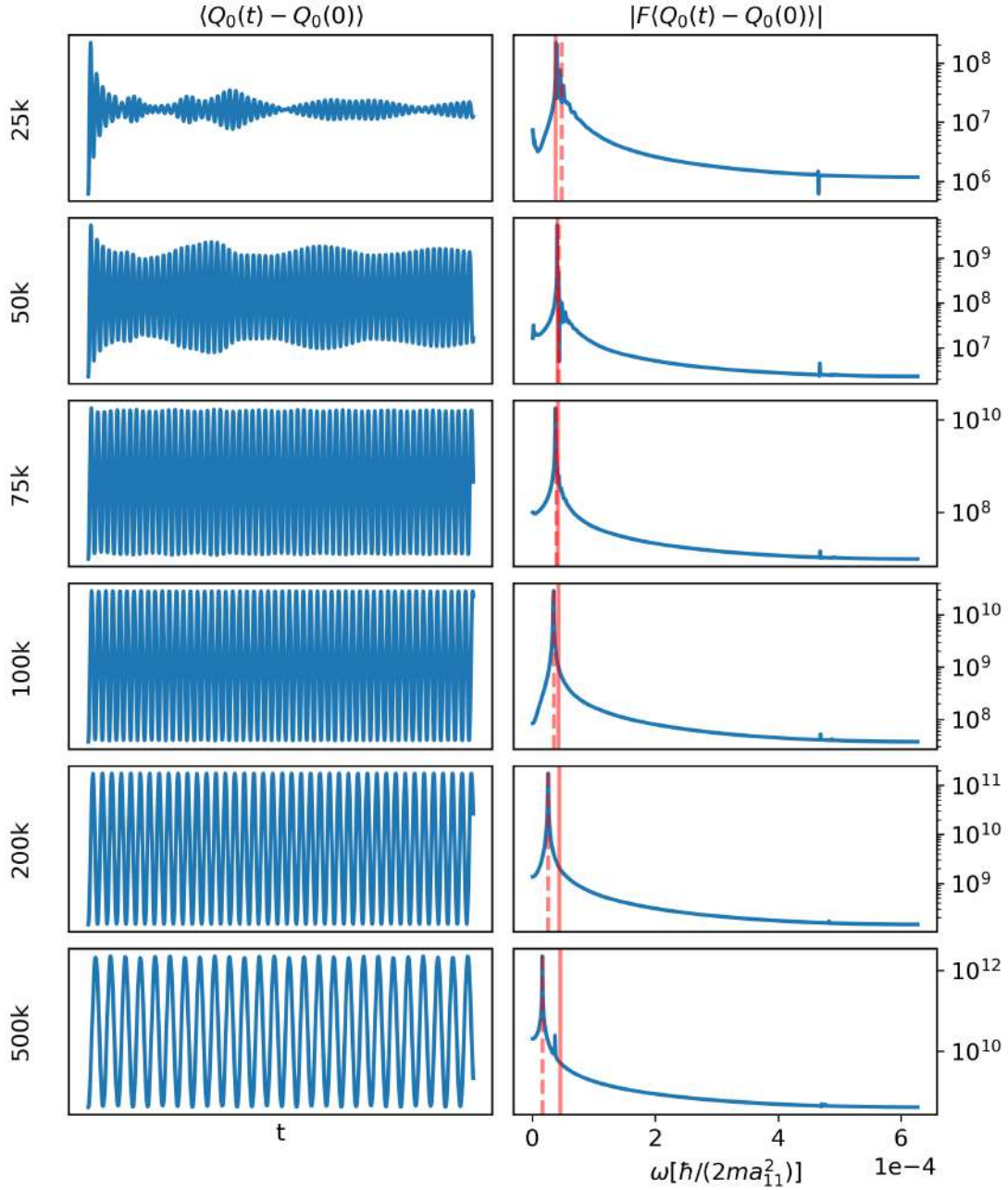


Figure 18: Time evolution of the monopole moment oscillations $\langle Q_0(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.10), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 0.50$.

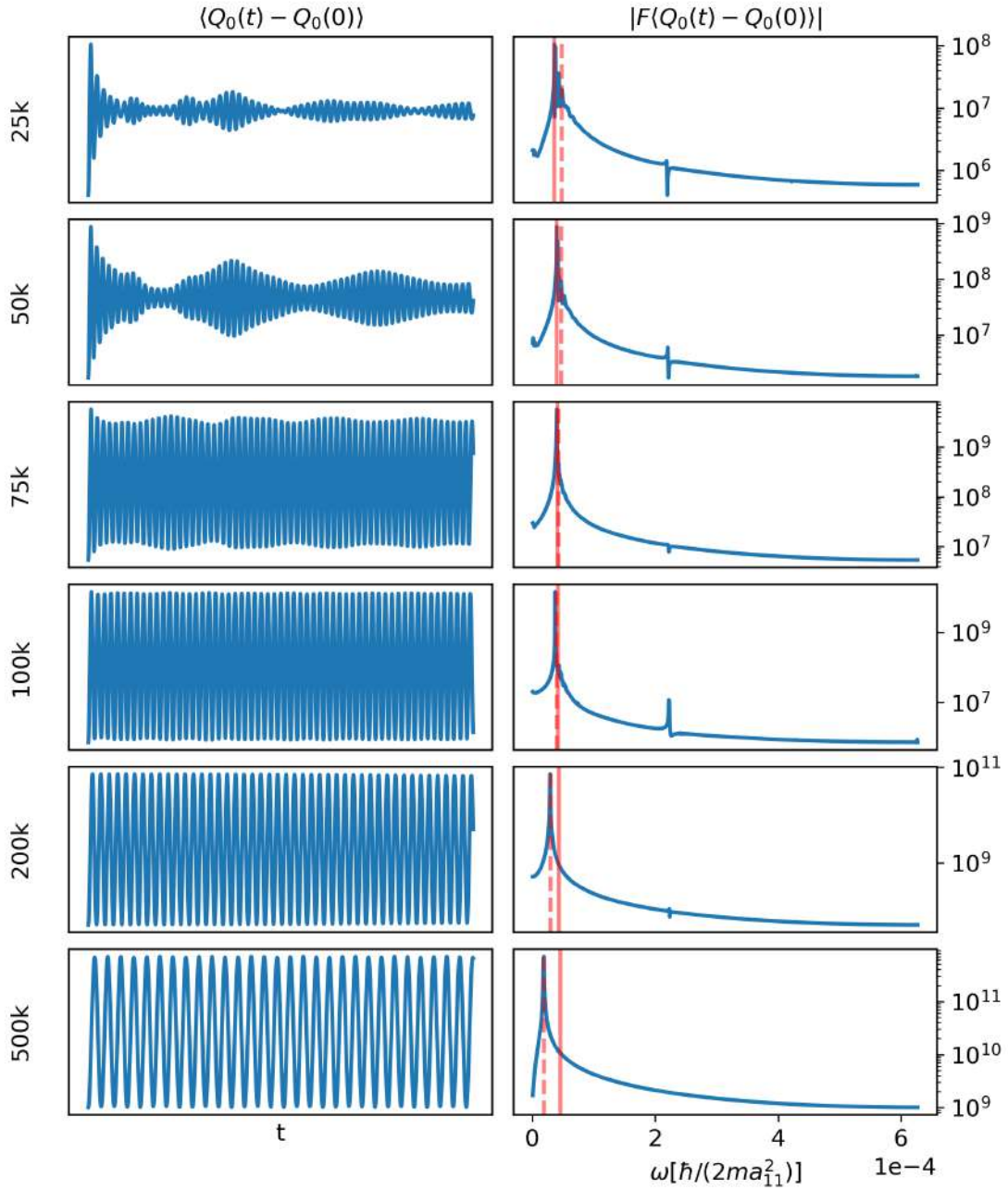


Figure 19: Time evolution of the monopole moment oscillations $\langle Q_0(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.10), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 0.75$.

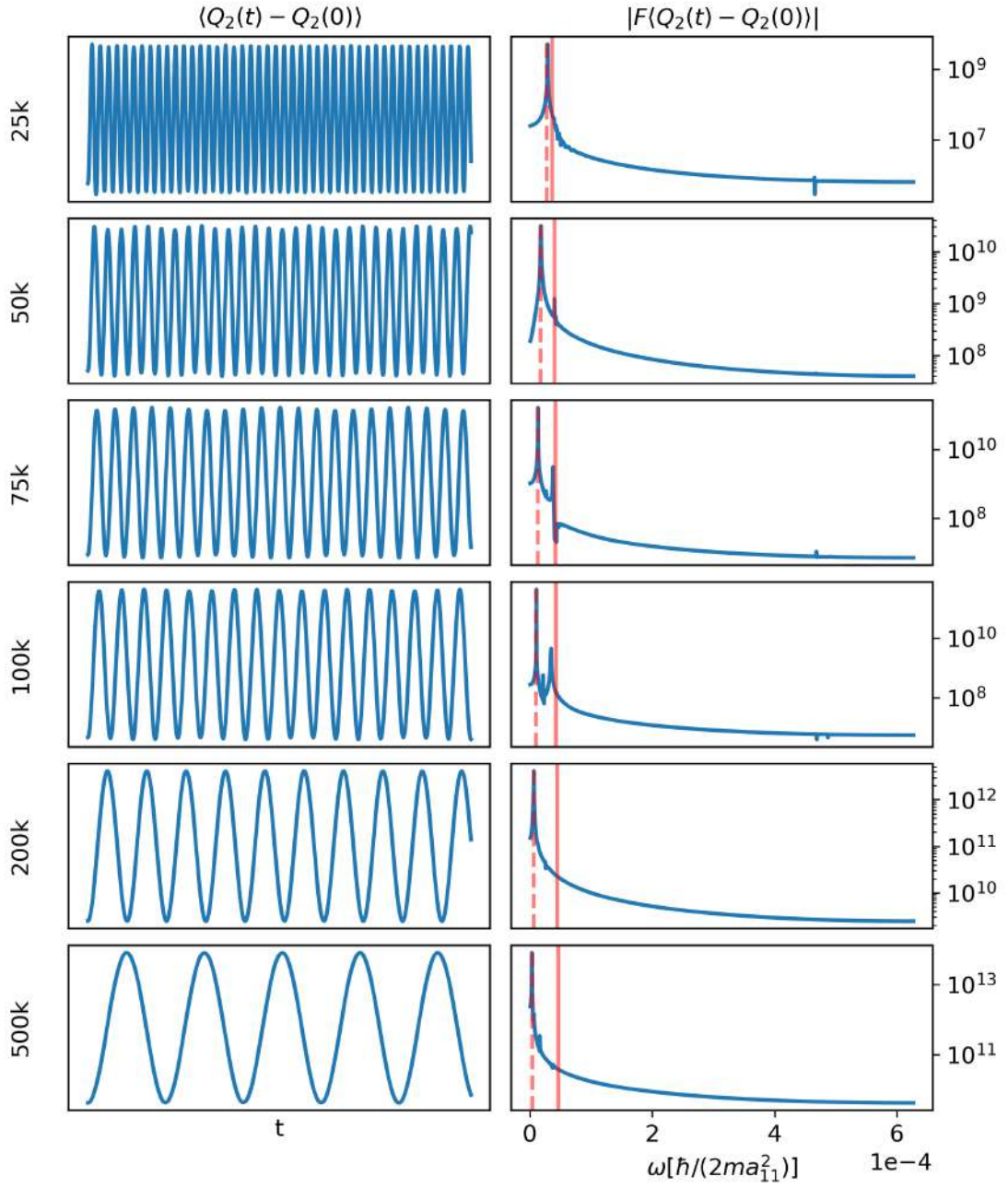


Figure 20: Time evolution of the quadrupole moment oscillations $\langle Q_2(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.11), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 0.50$.

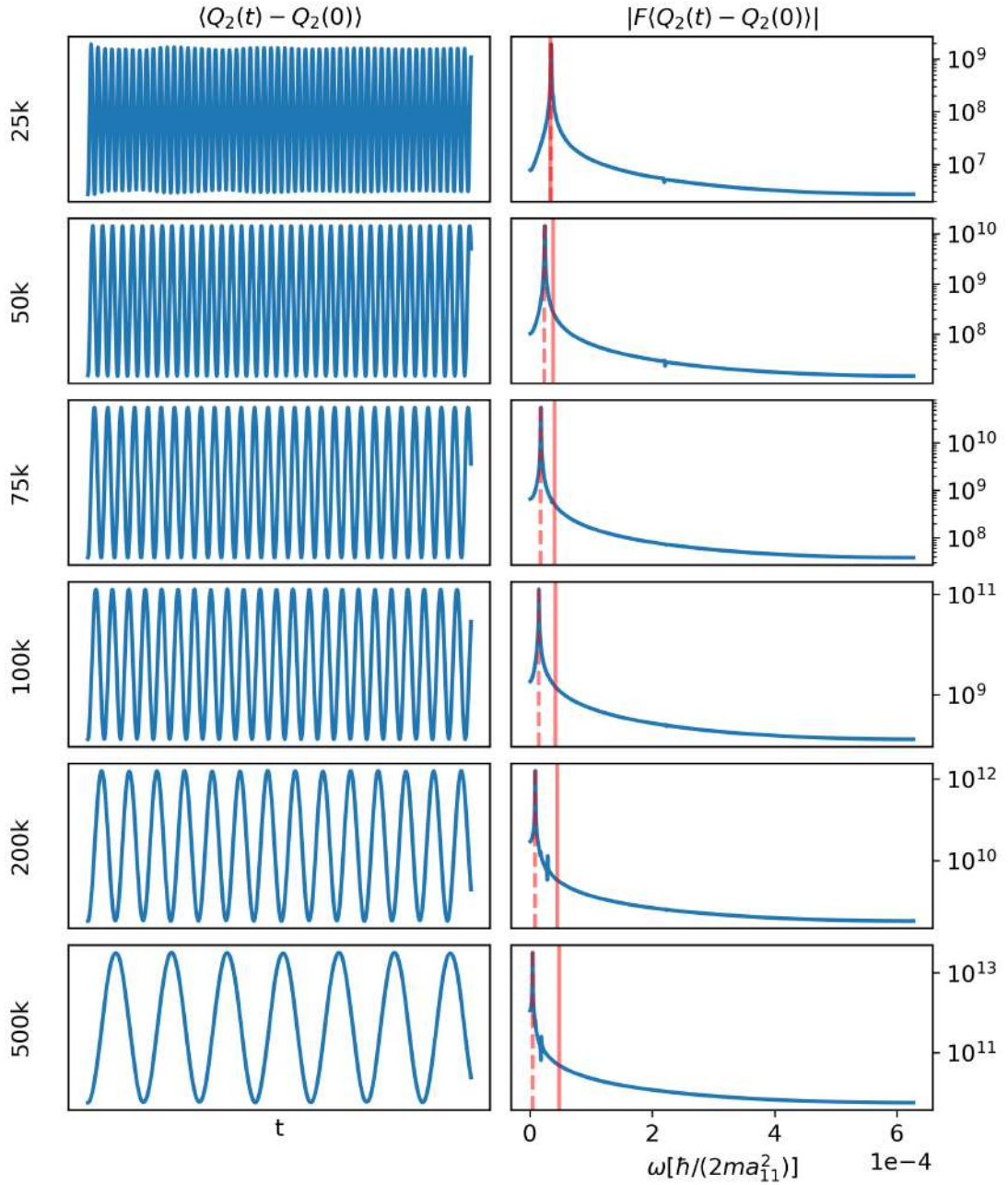


Figure 21: Time evolution of the quadrupole moment oscillations $\langle Q_2(t) \rangle$ (left) obtained by the QMC energy functional, and the corresponding frequency spectrum (right) obtained by the Fourier transform. In the right figures, the vertical red dashed lines correspond to the frequency $E_1/\hbar$ obtained by the sum rule in Eq. (3.11), and the vertical red solid lines correspond to the frequency $|\mu|/\hbar$. The squeezing parameter is $f = 0.75$.