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Self-bound droplet formation in two coupled Bose-Einstein condensates

Emerson Evaristo Chiquillo Márquez

Advisor

Professor *Sadhan Kumar Adhikari*

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SELF-BOUND DROPLET FORMATION IN TWO COUPLED BOSE-EINSTEIN CONDENSATES

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Comissão Examinadora:

Prof. Dr. SADHAN KUMAR ADHIKARI(Orientador)
Instituto de Física Teórica/UNESP

Prof. Dr. LAURO TOMIO
Instituto de Física Teórica/UNESP

Prof. Dr. GASTÃO INÁCIO KREIN
Instituto de Física Teórica/UNESP

Prof. Dr. ARNALDO GAMMAL
Instituto de Física da Universidade de São Paulo/IFUSP

Prof. Dr. TOBIAS FREDERICO
Instituto Tecnológico de Aeronáutica/ITA

Conceito: Aprovado

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"... No olvides lo aprendido,
no dejes de comprender.
Rodéate de buenos y tú lo parecerás.
Rodéate de sabios y algo en ti se quedará ... "

La danza del fuego, Mägo de Oz

"Una persona inteligente
resuelve un problema.
Una persona sabia,
lo evita!"

Albert Einstein

Resumo

O tema principal deste trabalho é pesquisar a formação estável de gotas em gases bosônicos acoplados, considerando alguns elementos extras àqueles já conhecidos na descrição das gotas convencionais. Para atingir esse objetivo, o estudo é feito principalmente por meio de uma teoria quântica de campos efetiva no formalismo da integral de trajetória. Para garantir que os resultados físicos sejam finitos, também usamos alguns aspectos básicos da renormalização por contratermos, incluindo métodos de regularização. Assim, estabelecemos descobertas em relação às gotas com correções não universais para as interações, em três, duas e uma dimensão, tanto em temperatura zero quanto finita. Em tres dimensões incluímos gotas com o acoplamento de Rabi e correções não universais para as interações em temperatura zero. Gotas em dois condensados de Bose-Einstein acoplados com interações dipolo-dipolo tanto em temperatura zero quanto finita também são exploradas.

Palavras Chaves: Bose-Bose gases; flutuações Gaussianas; gotas quânticas.

Áreas do conhecimento: Teoria da matéria condensada; condensação de Bose-Einstein; teoria quântica de campos.

Abstract

The main subject of this work is research the stable formation of droplets in Bose-Bose gases considering some extra elements to those already known in the description of conventional droplets. To this end, the study is carried out mainly through an effective quantum field theory in the the path-integral formalism. To ensure that the physical results are finite, we also use some basic aspects of renormalization by counterterms including regularization methods. So, we set key findings regarding to droplets with nonuniversal corrections to the interactions, in three, two, and one dimension, both at zero and finite temperature. We include three-dimensional Rabi-coupled droplets with nonuniversal corrections to the interactions at zero temperature. Droplets in two coupled Bose-Einstein condensates with dipole-dipole interactions both at zero and finite temperature are also explored.

Key-words: Bose-Bose gases; Gaussian fluctuations; quantum droplets.

Areas: Condensed matter theory; Bose-Einstein condensation; quantum field theory

Contents

Introduction **1**

1 Two coupled bosonic gases with nonuniversal corrections to the interactions: a droplet phase **5**

1.1 Introduction 6
1.2 Model and preliminaries 8
1.2.1 An effective-field theory for interacting bosons 8
1.2.2 Mean-field approximation to the grand-potential 12
1.2.3 Gaussian fluctuations to the grand-potential 12
1.2.4 Equal coupling constants considerations 14
1.3 Three-dimensional model 14
1.3.1 Three-dimensional finite-temperature effects 23
1.4 Two-dimensional model 24
1.4.1 Two-dimensional finite-temperature effects 29
1.5 One-dimensional model 30
1.5.1 One-dimensional finite-temperature effects 34
1.6 Summary and outlook 35

2 Droplets in Rabi-coupled nonuniversal Bose-Einstein condensates **37**

2.1 Introduction 37
2.2 An effective-field theory for Nonuniversal Rabi-coupled bosons . . 40
2.2.1 Mean-field ground states 43
2.3 Gaussian fluctuations of the symmetric ground-state 46
2.3.1 Gaussian fluctuations in absence of the nonuniversal corrections to the interactions 46
2.3.2 Gaussian fluctuations including the nonuniversal corrections to the interactions 54
2.3.3 Nonuniversal droplet phase 58
2.4 Summary and outlook 63

3 Droplets in two coupled dipolar Bose-Einstein condensates **64**

3.1 Introduction 64

3.2 Model and preliminaries . . . 67
3.3 Zero-temperature results . . . 69
3.3.1 Mean-field approximation to the grand-potential . . . 69
3.3.2 Gaussian fluctuations to the grand-potential . . . 70
3.3.3 Equal coupling constants . . . 72
3.4 Finite-temperature results . . . 78
3.5 Summary and outlook . . . 81

Conclusions **82**

A Path integral in quantum mechanics **84**
A.1 Path integral in phase space . . . 84
A.2 Path integral in configuration space . . . 86
A.3 Correlation functions . . . 86
A.4 Euclidean formulation of quantum mechanics . . . 88
A.5 Quantum-mechanical statistical partition function and correlation functions . . . 89
A.6 Path integrals from quantum mechanics to quantum field theory . 90

B Gaussian fluctuations **91**

C The coupling constants **95**
C.1 The two-body problem . . . 95
C.2 Partial waves decomposition . . . 96
C.3 On-shell approximation . . . 96

D Renormalization by counterterms and regularization methods **98**
D.1 Dimensional regularization . . . 98
D.2 Two-dimensional renormalization by counterterms . . . 99

E Fourier transform for the dipole-dipole interaction **103**
E.1 First method . . . 103
E.2 Second method . . . 104

References **107**

Introduction

In the early days of quantum mechanics the description of a new and intriguing physical phenomenon was proposed for the first time, the Bose-Einstein condensation (BEC). Proposed initially between 1924 and 1925 by Satyendra Nath Bose, who presented a novel way of counting states as an alternative to the established Boltzmann distribution of particles in the explanation of the spectrum of the black-body radiation for photons [1]. Shortly after, Albert Einstein based on this work and extending this idea to a gas of noninteracting massive atoms, predicts the presence of a phase transition below a critical temperature [2]. As a result of these works, particles with integer spin should occupy the same and lowest energy single particle state below the appropriate temperature, leading to the emergence of a coherent and a collective dynamical behavior. This new state of matter is known as the *Bose-Einstein condensation*, and it is a clear consequence of quantum statistical effects. In other words, at lower temperatures the de Broglie wavelength turns comparable to the distance between atoms, the quantum nature of the particles becomes relevant and each particle can be described by a localized wave-packet. Below a critical temperature, the wave-packet of each boson begins to overlap with the next one, and the next one, and the next one, and so on, until reaching zero temperature, where all of these bosons occupy the same quantum ground-state and this degenerate state is represented by an unique macroscopic wavefunction, the Bose-Einstein condensate wavefunction [3]. It is worth mentioning that in addition to the low temperature condition, the stable formation of a condensate needs a dilute system to reduce the three body collisions. These can destroy the ground-state, since these increases the kinetic energy giving rise to a heating and hence losses which depend on the atomic density. Therefore, only collisions between two particles are relevant, where the scattering length is much less than the interparticle spacing. However, it was necessary to wait for 70 years before a concrete experimental realization was obtained. It was achieved in 1995, combining different cooling techniques mostly developed since 70s. The density and temperature required to observe a BEC were reached in weakly-interacting dilute gases of ^{87}Rb [4], ^{7}Li [5], and ^{23}Na [6], (although in addition to the BEC formation the first evidence of collapse was also achieved in Ref. [5], curiously only Cornell, Wieman and Ketterle, co-authors in the other two works, were awarded with the Nobel prize in physics in 2001). From that moment on, ultracold atomic gases have been provided an excellent environment for studying quantum many-particle systems.

So, just over a century after the prediction of Bose-Einstein condensation and thirty years after the experimental realization, science has been and continues to be a witness of the impact caused by such a phenomenon. See Ref. [7] for a recent historical overview of the different fields of research where the BEC appears, we briefly mention some of these. One of the first insight associated to the emergence of physics of BEC in other fields of research is related to BCS (Bardeen-Cooper-Schrieffer) theory, which is widely used in the understanding of the superconductivity. Currently this connection has been established in terms of the crossover from a BEC to a BCS-like state of weakly bound fermion pairs [8, 9, 10]. We also have BECs of exciton-polaritons, arising from photons confined in microcavities and the strong coupling of excitons confined in quantum wells [11]. Another notable development includes the synthetic generation of non-Abelian gauge fields in neutral mixtures of BECs by means of laser beams [12, 13, 14]. The BEC phenomenon is also believed to occur in fields as varied as, high-energy physics, astrophysics, and cosmology. For example, the development in exciton-polaritons BECs has allowed lead to controllable studies of analogous gravitational phenomena [15], which are proposals for gravitational theories that might share properties with the BECs. For instance we have the creation of an analog of a black hole in a BEC [16], or the study of the dynamics of a supersonically expanding ring-shaped BEC [17] to explored the physics of the cosmological expansion in the universe. Superfluidity in neutron stars may explain pulsar glitches through quantum vortices [18]. On a cosmological scale, the BEC formation and the superfluidity are considered as potential mechanisms for understanding dark matter [19, 20, 21]. Self-gravitating BECs are also considered [22]. All this seems to indicate some kind of ubiquity of the Bose-Einstein condensation in the quantum nature of the matter.

In the context of the condensed matter and more specifically in relation to the atomic three-dimensional attractive Bose-Bose condensates a new kind of ground-state was proposed in 2015 [23]. In a short time this idea was also considered in low dimensions [24]. This new state of matter has been named as *droplet* phase, or droplet for short, as it appears in most current literature. For its part, experimental evidence related to the existence of this phase was not long in coming, [25, 26, 27, 28, 29, 30, 31, 32]. Almost at the same time, this phenomenon was also found in BECs of highly magnetic atoms where the dipole-dipole interactions play a key role [33, 34, 35, 36, 37, 38, 39]. The long-range character and the anisotropy of these interactions give great phenomenological richness [40, 41, 42, 43]. To understand, in a general way, the physical principle behind this phenomenon, one must take into account the fact that a three-dimensional attractive BEC undergoes an instability by collapse [44, 45]. That means that there exist a threshold, determined by the interactions or the particle density, after which the condensate suffers an implosion. The same kind of instability can occur in condensed Bose-Bose mixtures or in dipolar BECs. However, including the correction coming from zero-point motion of Bogoliubov excitations, it is possible to avoid the collapse, achieving a stable ground-state: a liquidlike phase or droplet. In short, such a state is a result of an attraction-repulsion balance between the mean-field energy (leading contribution), and the energy coming from the first order in the fluctuations (sub-leading contribution). We emphasize that in low dimensionality or considering dipole-dipole interactions in BECs some small subtleties are present and are related to which term is attractive and which is repulsive, but the principle is the same, as we will see later in different parts of this work. In the research of droplets it is remarkable that comparing experimental and numerical results with theoretical predictions, some discrepancies have been found. For instance, a stable droplet formation requires a critical minimum number of atoms [25, 46, 47, 48] and this value is less than predicted in Ref. [23]. In addition and due to the sensitive nature of the fluctuations themselves the effect on these of some other parameters remains as an open issue. Since the description of droplets arises in a weakly-interacting regime, this is favorable from a theoretical framework because we can implement a perturbative treatment, where it is a well established fact that the applicability of perturbative calculations requires as a prerequisite the smallness of the coupling. So the droplets are a natural platform to implement such calculations in a systematic and well controlled fashion.

From the above mentioned, and in order to have a better understanding of fluctuations behavior on interacting Bose-Bose gases we research the effects of some extra ingredients. So this work has been written so that each chapter can be read independently and, it is organized as follows: the chapter 1 is devoted to research the effects of the nonuniversal corrections to the interatomic interaction potential both at zero- and finite-temperature. It is well known that in conventional bosonic gases the parameter characterizing the two-body interactions is given only in terms of the s-wave scattering length, in this case we have an universal regime, but if the physical quantities depend on properties other than the s-wave scattering length we have a nonuniversal regime [49]. We set conditions under which the formation and stability both at zero and finite temperature of a self-bound droplet with nonuniversal corrections to the interactions, in three, two and one dimension is favorable. In the chapter 2, the main subject is focused in research the existence of three-dimensional droplets at zero temperature with nonuniversal corrections to the interactions in Bose-Bose gases including also a coherent coupling between atomic internal states provided by a Rabi frequency. In the chapter 3 we consider the effect of the fluctuations in two coupled dipolar BECs. The analysis is focused on establish some relevant features under which the formation and stability of a droplet is possible. We also include results at finite-temperature, motivated by some recent experimental and numerical developments. Some conclusions are included in the final chapter. In order to facilitate the reading of the main aspects of the work, some technical details have been included in the different appendices.

The results achieved in the present study could be obtained by means of quantum mechanics [44, 45], in terms of usual bosonic creation and annihilation operators as in the seminal works [23, 24]. Nevertheless, we use an alternative but equivalent method, the path-integral formalism in the context of an effective quantum field theory (QFT). The goal of an effective QFT is to offer a treatment of the relevant degrees of freedom and the symmetries governing the dynamics of the system. Although path-integrals have their roots in the quantum mechanics, its main field of action has been in high energy physics as a key element in the development of the relativistic QFT. However the Bose-Einstein condensation as a scalar non-relativistic QFT can be studied with such a method [49]. We also emphasize that to deal with the infinities proper of the theory it is necessary to include some elements of renormalization by counterterms and regularization methods.

As a final comment, we mention that part of this work has been published in the following papers:

- E. Chiquillo, *Bose-Bose gases with nonuniversal corrections to the interactions: a droplet phase*, Ann. Phys. **475**, 169955 (2025).
- E. Chiquillo, *Nonuniversal equation of state for Rabi-coupled bosonic gases: a droplet phase*, Ann. Phys. **479**, 170071 (2025).

Chapter 1

Two coupled bosonic gases with nonuniversal corrections to the interactions: a droplet phase

Through an effective quantum field theory within Bogoliubov's framework and taking into account nonuniversal effects of the interatomic potential we analytically derive the leading Gaussian zero- and finite-temperature corrections to the equation of state of ultracold interacting Bose-Bose gases. We calculate the ground-state energy per particle at zero and low temperature for three- two- and one-dimensional two-component bosonic gases. By tuning the nonuniversal contribution to the interactions we address and establish conditions under which the formation and stability of a self-bound liquidlike phase or droplet with nonuniversal corrections to the interactions (DNUC) is favorable. At zero temperature in three-dimensions and considering the nonuniversal corrections to the attractive interactions as a fitting parameter the energy per particle for DNUC is in good agreement with some diffusion Monte Carlo results. In two dimensions the DNUC present small deviations regarding conventional droplets. For the one-dimensional DNUC the handling of the nonuniversal effects to the interactions achieves a qualitative agreement with the trend of some available Monte Carlo data in usual droplets. We also introduce some improved Gross-Pitaevskii equations to describe self-trapped DNUC in three, two and one dimension. We briefly discuss some aspects at low temperature regarding nonuniversal corrections to the interactions in Bose-Bose gases. We derive the dependencies on the nonuniversal contribution to the interactions but also on the difference between intra- and inter-species coupling constants. This last dependence crucially affect the three- and the two-dimensional DNUC driving thus to a thermal-induced instability. This thermal instability is also present in one-dimensional Bose-Bose gases, but it is not relevant on the formation of DNUC. This is explained because the necessary attraction mechanism to achieve this phase naturally arises in the fluctuations at zero temperature without major restrictions as it happens in the other dimensions. This chapter is based on Ref. [50].

1.1 Introduction

The highly nontrivial and subtle stabilization between the mean-field energy and the energy coming from the fluctuations in ultradilute Bose-Bose gases has attracted an increasing interest. Such a balance has given rise to the liquidlike phase or droplet phase, revealing thus the crucial role played by the fluctuations [23, 24]. This intriguing new state of matter lies in the mechanical stabilization of paradigmatic mean-field collapse threshold in a condensed Bose-Bose mixture through the first Gaussian correction coming from zero-point motion of Bogoliubov excitations. This proposal has allowed the birth of a fascinating and fast development research field [51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69]. Though the fluctuations are usually small and these are generally neglected, recent experimental achievements have put in evidence the outstanding influence of these small corrections on the equation of state for attractive Bose-Bose gases. The droplet phase has been obtained in homonuculear ^{39}K-^{39}K mixtures [25, 26, 27, 28] and heteronuclear ^{41}K-^{87}Rb mixtures [29]. Also has been studied the dynamical formation of self-bound droplets in an attractive mixture of ^{39}K atoms [30]. More recently the observation of a Lee-Huang-Yang (LHY) fluid in a ^{39}K spin mixture confined in a spherical trap potential has been achieved [31]. Droplets have been also obtained in a mixture of ^{23}Na and ^{87}Rb with tunable attractive inter-species interactions [32]. It is also worth mentioning that soon after the theoretical proposal of Bose-Bose droplets, this idea was extended to the context of one-component Bose gases with magnetic atoms [33, 34, 70, 71, 72, 73]. Experimental evidence of dipolar droplets existence with atoms of ^{164}Dy [35, 36, 37, 38] and ^{168}Er [39] was also discovered. However, it is remarkable that comparing experimental evidence with theoretical predictions, in both droplets in mixtures of Bose-Bose gases and droplets in bosonic dipolar gases, some discrepancies have been found. In fact, in three-dimensional Bose-Bose gases it was experimentally observed that a stable droplet formation requires a critical minimum number of atoms [25]. This critical value is less than predicted by the proposed model in Ref. [23]. Some differences are also present comparing the theoretical model with numerical results obtained by means of Monte Carlo methods [46, 47, 48]. Therefore, given the discrepancy between the theoretical model and both experimental and numerical results, it is necessary to find a model that allows a better description of this phenomenon. In an attempt to achieve this, a phenomenological and beyond LHY framework has been developed in Ref. [74] for three- and one-dimensional Bose-Bose droplets.

From a general theoretical framework, such a droplet phase in both two-component ultracold Bose gases and dipolar bosonic gases remains weakly interacting, allowing thus for a theoretical perturbative treatment. A key ingredient in Bose-Bose droplets description is to consider the weakly interatomic interactions approximated by a local contact interaction. In this sense, only one parameter characterizes the two-body interactions and it is encoded in an effective theory in terms of the s-wave scattering length a. This unique dependence is considered as an universal regime [49]. On the other hand, the fact that physical quantities depend on properties other than the s-wave scattering length is considered as a nonuniversal regime. In addition and due to the sensitive nature of the fluctuations themselves the effect on these of some other parameters remains as an open issue. Therefore for a better understanding of fluctuations behavior on interacting Bose-Bose mixtures and motivated by the enhanced role of these, we consider an extra ingredient. We propose a step beyond by researching the effect of the nonuniversal corrections to the interatomic interaction potential [75]. We address and focused theoretically on formation and stability of self-bound Bose-Bose droplets with nonuniversal corrections to the interactions (DNUC) both at zero and low temperature. We consider DNUC in three- two- and one-dimension. Thermal corrections on mixtures of two-component bosonic gases with zero-range interactions have been studied in Ref. [51] (see also [54]). Recently, the implementation of Monte Carlo algorithms has been carried out in the study of finite temperature in Bose-Bose mixtures [76, 77, 78]. We stress that although in recent years have been included nonuniversal corrections to the interactions on the study of the equation of state in one-component Bose gases in three [79], two [80] and one dimension [81], the necessary conditions for a droplet formation have not been considered.

The rest of the chapter is organized as follows. In Section 1.2 we introduce an effective-field theory for interacting bosons taking into account nonuniversal corrections to the interactions. We also bring up some elements of interest in the path-integral formalism which are employed to obtain the equation of state of two-component bosonic gases with nonuniversal corrections to the interactions in dimension d, with $d = 3, 2, 1$. This formalism is widely used in relativistic quantum field theory (QFT), and almost any book on QFT covers this topic in great detail. However, the path integral can be also considered in the study of ultracold gases [49, 82]. In appendix A we include some aspects aimed at readers unfamiliarized with this formalism. The appendix is focused in the context of quantum mechanics, which is where this method arises, but the extension to the study of ultracold gases is expected. In other words we only consider some aspects of interest for this work related to a scalar non-relativistic QFT. So, we derive the mean-field grand-canonical potential. We also obtain general expressions for the grand-canonical potential dealing with fluctuations and thermal effects. In order to simplify the problem and to know some insights into the underlying physics of the DNUC we consider a symmetric scenario. To keep the notation as simple as possible, in all dimensions we use a for the scattering length and r for the effect of the nonuniversal contribution to the interactions, respectively. After establishing some initial aspects, we calculate and analyze the existence conditions of stable $3d$ DNUC at zero and finite temperature in section 1.3. We present two different equations of state each related to two different expansions of the phase shift in $3d$ scattering theory. In section 1.4 we investigate the stable formation of $2d$ DNUC. We also include finite-temperature corrections. In section 1.5 we present the formation of stable $1d$ DNUC at zero and finite temperature. In this section we also discuss some interesting differences regarding $2d$ and $3d$ DNUC. In section 1.6 we draw a final discussion and we present some future perspectives of our results.

1.2 Model and preliminaries

1.2.1 An effective-field theory for interacting bosons

At theoretical level, in the regime of low-momentum expansion of the interaction potential some improvements to obtain useful and analytical expressions describing ultracold bosons have been proposed. In a first attempt within the framework of an effective field theory, the next-to-leading effects of the interactions in homogeneous three-dimensional Bose-Einstein condensates are calculated in Ref. [75]. An effective Lagrangian constrained by the symmetries of the original Lagrangian, namely, Galilean invariance, parity, and time reversal, is considered. The coefficients of this Lagrangian are determined by imposing that the effective theory reproduces the amplitude for low-energy atom-atom scattering up to errors that scale like the square of the energy. Going to the center of momentum frame, using the energy conservation and regularization prescriptions, the exact T-matrix element can be determined analytically. Thus the scattering length and the nonuniversal corrections for the s-wave scattering are defined by the expansion of the phase shift. On the other hand, in Refs. [83, 84, 85] the next-to-leading order term in the low-momentum expansion of the interaction potential is obtained based on the calculation of the energy shift due to a phase shift in the wavefunction. We stress that due to the different considerations employed, the two above approaches do not coincide with each other. In particular, in the last approximation if the nonuniversal correction goes to zero some finite contributions of the scattering length still, and we not obtain the conventional dependence on the scattering length. It is worth noting that the improvement developed in Ref. [75] has been employed in recent years to study the effects of the nonuniversal contribution to the interactions in the equation of state of bosonic gases in three dimensions [79], with results in good agreement with Monte Carlo calculations. Such a effective field theory has been also adopted in two [80] and one dimension [81]. So we consider the effective field theory approach from Ref. [75]. Our motivation lies in the fact that this procedure is directly related to the scattering theory by means of the T-matrix. Furthermore when the nonuniversal effects vanishes we recover the widely known results in the study of bosons and employed in Bose-Einstein condensation research. Additionally we can also extent the idea to lower dimensions. So we consider a formalism reasonably suitable to study an effective field theory for ultracold bosons. In order to establish the effective Lagrangian for two component bosonic gases with nonuniversal corrections to the interactions, for simplicity, we first consider one-component Bose gases. After that, we adopt the natural extension to two-component bosonic gases.

In the path-integral formalism we consider interacting and identical bosons of mass m with chemical potential μ in a d-dimensional, $(d = 3, 2, 1)$, box of volume L^d with the Lagrangian density given by

$$\begin{aligned} \mathcal{L} &= \psi^*(\mathbf{r},\tau)\Big(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 - \mu\Big)\psi(\mathbf{r},\tau) \\ &+ \frac{1}{2}\int d^d r' |\psi(\mathbf{r}',\tau)|^2 V(|\mathbf{r}-\mathbf{r}'|)|\psi(\mathbf{r},\tau)|^2. \end{aligned} \tag{1.1}$$

The fields are considered at position $\mathbf{r}$ and imaginary time τ, and $V(|\mathbf{r}-\mathbf{r}'|)$ is the two-body interaction potential between bosons. Dealing with ultracold and dilute bosons, the most common scheme to taking into account interaction effects is replacing $V(r)$ (where $r \equiv |\mathbf{r}-\mathbf{r}'|$), adopting an approximated zero-range Fermi pseudo-potential $V^{(0)}(r) = g^{(0)}\delta^{(d)}(r)$. The specific form of the strength of the interaction $g^{(0)}$ depends on the dimension of the system. At the moment the most relevant aspect of this term is that it only depends on the scattering length a. An improvement of the zero-range approximation can be achieved by replacing the Fourier transform of the interaction potential $\widetilde{V}(k) = \int d^d r \exp{(\mathrm{i}\mathbf{k}\cdot\mathbf{r})} V(r)$ with the pseudo-potential $\widetilde{V}(k) = g^{(0)} + g^{(2)}k^2$. This is obtained as the Taylor expansion in k around $k=0$ of $\widetilde{V}(k)$ up order two. So we have $g^{(0)} = \widetilde{V}(0)$, and $g^{(2)} = (1/2)\widetilde{V}''(k)|_{k=0}$. Since $k=0$ is a minimum of the potential, the linear contribution in the Taylor expansion vanishes. By means of the inverse Fourier transform of the pseudo-potential $\widetilde{V}(k)$, the pseudo-potential in real space is used into the second line of Eq. (1.1), and we get the following effective Lagrangian density including effective nonuniversal effects of the interactions

$$\begin{aligned} \mathcal{L} &= \psi^*(\mathbf{r},\tau)\Big(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 - \mu\Big)\psi(\mathbf{r},\tau), \\ &+ \frac{1}{2}g^{(0)}|\psi(\mathbf{r},\tau)|^4 - \frac{1}{2}g^{(2)}|\psi(\mathbf{r},\tau)|^2\nabla|\psi(\mathbf{r},\tau)|^2. \end{aligned} \tag{1.2}$$

Like $g^{(0)}$, the strength of the nonuniversal effects to the interactions $g^{(2)}$ also depends on the spatial dimension of the system and the specific form will be discussed later.

By considering the natural extension of the procedure outlined above we consider two-component interacting ultracold Bose gases. Each component is described by a complex bosonic field ψ_α ($\alpha = 1,2$) with equal-mass m, and chemical potentials μ_α. The effective Euclidean Lagrangian density in a d-dimensional box of volume L^d is given by

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}^{(0)}_{\text{int}} + \mathcal{L}^{(2)}_{\text{int}}, \tag{1.3}$$

where

$$\mathcal{L}_0 = \sum_{\alpha=1,2}\Big[\psi^*_\alpha(\mathbf{r},\tau)\Big(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 - \mu_\alpha\Big)\psi_\alpha(\mathbf{r},\tau)\Big], \tag{1.4}$$

$$\mathcal{L}^{(0)}_{\text{int}} = \frac{1}{2}\sum_{\alpha,\sigma=1,2} g^{(0)}_{\alpha\sigma}|\psi_\alpha(\mathbf{r},\tau)|^2|\psi_\sigma(\mathbf{r},\tau)|^2, \tag{1.5}$$

and,

$$\mathcal{L}_{\text{int}}^{(2)} = -\frac{1}{2} \sum_{\alpha,\sigma=1,2} g_{\alpha\sigma}^{(2)} |\psi_\alpha(\mathbf{r},\tau)|^2 \nabla^2 |\psi_\sigma(\mathbf{r},\tau)|^2. \tag{1.6}$$

The specific form of the couplings will defer further discussion until addressing each dimension separately. The strength of the zero-range interactions is expressed through the intra- and interspecies coupling constants $g_{\alpha\alpha}^{(0)}$ and $g_{\alpha\sigma}^{(0)}$, respectively. The role played by the effects beyond the zero-range approximation to the interactions is encoded in expression (1.6). Thus we have the coupling constants for intra-species and inter-species considering the nonuniversal corrections to the interactions $g_{\alpha\alpha}^{(2)}$ and $g_{\alpha\sigma}^{(2)}$, respectively.

In order to obtain the ground state of the system, we calculate the grand potential $\Omega = -k_B T \log \mathcal{Z}$. In the path-integral formalism the grand canonical partition function $\mathcal{Z}$ of the system at temperature T is written as $\mathcal{Z} = \int \mathcal{D}[\Psi,\Psi^*] \exp(-S[\Psi,\Psi^*]/\hbar)$, and it is governed by the action

$$S[\Psi,\Psi^*] = \int_0^{\hbar\beta} d\tau \int_{L^d} d^d r \mathcal{L}[\Psi,\Psi^*], \tag{1.7}$$

with $\Psi = (\psi_1, \psi_2)^T$, $\beta = (k_B T)^{-1}$, k_B the Boltzmann constant, $d = 3,2,1$, and $\mathcal{L}$ given by Eq. (1.3).

At zero temperature we assume the bosons condensate into the zero-momentum states. Although strictly Bose-Einstein condensation is prevented in low dimensionality, a finite-size system at sufficiently low temperature allows for a quasicondensation [86, 87]. In order to perform a perturbative expansion we set $\psi_\alpha(\mathbf{r},\tau) = \phi_\alpha + \eta_\alpha(\mathbf{r},\tau)$. Where $\phi_\alpha \equiv \langle \psi_\alpha(\mathbf{r},\tau) \rangle$ [88], corresponds to the macroscopic condensate ($3d$) or quasicondensate ($2d$, and $1d$) wave-function. The fluctuations around ψ_α are given by $\eta_\alpha(\mathbf{r},\tau)$ and these are orthogonal to the condensate (quasicondensate) of the same species [88, 89]. Since here the relative phases of the wave-functions do not play a role, we have $n_\alpha = |\phi_\alpha|^2 = N_\alpha / L^d$, as the density of particles or condensate (quasicondensate) density in the mean-field approximation. Since ϕ_α describes the condensate (quasicondensate), the linear terms in the fluctuations vanish such that ϕ_α really minimizes the action [88]. Therefore results in the mean-field approximation could be obtained by minimizing the mean-field grand potential Ω_0 with respect to ϕ, as will be seen later. Now, by expanding the action up to the second order (Gaussian) in $\eta_\alpha(\mathbf{r},\tau)$ and $\eta_\alpha^*(\mathbf{r},\tau)$, we arrive at the split grand potential $\Omega = \Omega_0 + \Omega_{\text{GF}}$. Where Ω_0 is the mean-field grand potential, while Ω_{GF} takes into account both zero- and finite-temperature fluctuations to the grand-potential.

1.2.2 Mean-field approximation to the grand-potential

At first instance we carry out the analysis of the mean-field contribution to the grand-potential, from which we get the following

$$\frac{\Omega_0}{L^d} = \sum_{\alpha=1,2} \Big(-\mu_\alpha \phi_\alpha^2 + \frac{1}{2} \sum_{\sigma=1,2} g_{\alpha\sigma}^{(0)} \phi_\alpha^2 \phi_\sigma^2 \Big), \tag{1.8}$$

which is not dependent on the nonuniversal effects to the interaction, given the derivative term of $\mathcal{L}_{\mathrm{int}}^{(2)}$. So by minimizing Ω_0 with respect to ϕ_α, such that $\partial \Omega_0 / \partial \phi_\alpha = 0$, we obtain [51], $\mu_\alpha = g_{\alpha\alpha}^{(0)} \phi_\alpha^2 + g_{\alpha\sigma}^{(0)} \phi_\sigma^2$, with $\alpha, \sigma = 1,2$ and $\alpha \neq \sigma$. Hence the mean-field grand potential becomes

$$\frac{\Omega_0}{L^d} = -\frac{1}{2} \sum_\alpha \frac{g_{\sigma\sigma}^{(0)} \mu_\alpha^2 - g_{\alpha\sigma}^{(0)} \mu_\alpha \mu_\sigma}{g_{\alpha\alpha}^{(0)} g_{\sigma\sigma}^{(0)} - \big[g_{\alpha\sigma}^{(0)} \big]^2} \tag{1.9}$$

1.2.3 Gaussian fluctuations to the grand-potential

The grand potential of the Gaussian fluctuations Ω_{GF} is provided by (see appendix B, and [82])

$$\Omega_{\mathrm{GF}} = \frac{1}{2\beta} \sum_{k>0} \sum_{n=-\infty}^{+\infty} \ln \det [\mathbb{G}^{-1}(k, \omega_n)], \tag{1.10}$$

with the bosonic Matsubara's frequencies $\omega_n = 2\pi n / (\hbar\beta)$, and the 4×4 inverse fluctuation propagator $\mathbb{G}^{-1}$ given as

$$\mathbb{G}^{-1} = \begin{pmatrix} \mathbf{G}_{11}^{-1} & \mathbf{G}_{12}^{-1} \\ \\ \mathbf{G}_{12}^{-1} & \mathbf{G}_{22}^{-1} \end{pmatrix}, \tag{1.11}$$

with the symmetric 2×2 matrices

$$\mathbf{G}_{11}^{-1} = \begin{pmatrix} -i\hbar\omega_n + \epsilon_k + h_{11} & (g_{11}^{(0)} + g_{11}^{(2)} k^2) \phi_1^2 \\ \\ (g_{11}^{(0)} + g_{11}^{(2)} k^2) \phi_1^2 & i\hbar\omega_n + \epsilon_k + h_{11} \end{pmatrix}, \tag{1.12}$$

$h_{11} = (2g_{11}^{(0)} + g_{11}^{(2)}k^2)\phi_1^2 + g_{12}^{(0)}\phi_2^2 - \mu_1$, $\mathbf{G}_{22}^{-1} = \mathbf{G}_{11}^{-1}(1 \leftrightarrow 2)$, and

$$\mathbf{G}_{12}^{-1} = (g_{12}^{(0)} + g_{12}^{(2)}k^2)\phi_1\phi_2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{1.13}$$

By solving the determinant of the inverse propagator we get

$$\Omega_{\mathrm{GF}} = \frac{1}{2\beta} \sum_{\substack{k>0 \\ n=-\infty}}^{+\infty} \ln\left[(\hbar^2\omega_n^2 + E_+^2)(\hbar^2\omega_n^2 + E_-^2)\right], \tag{1.14}$$

with the zero-point energy of collective excitations or Bogoliubov spectra given as

$$E_\pm(k, \mu_1, \mu_2) = [\epsilon^2(k) + \epsilon(k) f(\mu_1, \mu_2)]^{1/2}, \tag{1.15}$$

with the free-particle energy $\epsilon(k) = \hbar^2 k^2/2m$, and

$$f(\mu_1, \mu_2) = \frac{1}{\Delta_-}\left(\tau_+ \pm \sqrt{\tau_-^2 + 4\Lambda}\right), \tag{1.16}$$

where $\tau_+ = f_2^- \mu_1 + f_1^- \mu_2, \tau_- = f_2^+ \mu_1 - f_1^+ \mu_2$, $\Lambda = h^2(\Delta_+ \mu_1\mu_2 - h_2\mu_1^2 - h_1\mu_2^2)$, $\Delta_\pm = g_{11}^{(0)} g_{22}^{(0)} \pm [g_{12}^{(0)}]^2$, $h = g_{12}^{(0)} + g_{12}^{(2)}k^2$, $h_1 = g_{11}^{(0)} g_{12}^{(0)}$, $h_2 = g_{22}^{(0)} g_{12}^{(0)}$, $f_1^\pm = g_{11}^{(0)}(g_{22}^{(0)} + g_{22}^{(2)}k^2) \pm g_{12}^{(0)}(g_{11}^{(0)} + g_{11}^{(2)}k^2)$, $f_2^\pm = f_1^\pm(1 \leftrightarrow 2)$. The sum over the bosonic Matsubara's frequencies given by Eq. (1.10) can be read as $\Omega_{\mathrm{GF}} = \Omega_{\mathrm{GF}}^{(0)} + \Omega_{\mathrm{GF}}^{(T)}$ [82, 90], such that

$$\Omega_{\mathrm{GF}}^{(0)} = \frac{1}{2}\sum_{k,\pm} E_\pm(k), \tag{1.17}$$

represents the Gaussian fluctuations at zero temperature, and,

$$\Omega_{\mathrm{GF}}^{(T)} = \frac{1}{\beta}\sum_{k,\pm} \ln\left(1 - e^{-\beta E_\pm(k)}\right), \tag{1.18}$$

considers the thermal Gaussian fluctuations. For now we will leave this last contribution aside and we focus on results at zero temperature. However, we will return to thermal effects up later. In the continuum limit $\sum_k \to L^d \int d^dk/(2\pi)^d$, the contribution of the zero-temperature Gaussian fluctuations to the ground-state can be read as

$$\frac{\Omega^{(0)}_{\mathrm{GF}}}{L^d} = \frac{S_d}{2}\sum_{\pm}\int_0^\infty \frac{dk}{(2\pi)^d}\, k^{d-1}E_\pm, \tag{1.19}$$

with $S_d = 2\pi^{d/2}/\Gamma(d/2)$ the solid angle in d dimensions and $\Gamma(x)$ the Euler gamma function. It is worth mentioning that although this integral is ultraviolet divergent at $d = 3, 2, 1$, it is possible to obtain finite results avoiding this issue by means of regularization methods [82, 91, 92].

1.2.4 Equal coupling constants considerations

In order to obtain closed analytical expressions useful simplifications take place when the intra-species and the nonuniversal coupling constants are equal, such that, $g^{(0)}_{11} = g^{(0)}_{22} = g^{(0)}$ and, $g^{(2)}_{11} = g^{(2)}_{22} = g^{(2)}$. In addition we take the same density in different species $n_1 = n_2 = n/2$. Given these considerations, it is natural to take the same chemical potential, $\mu_1 = \mu_2 = \mu$. From these simplifications we get the following mean-field grand potential

$$\frac{\Omega_0}{L^d} = -\frac{\mu^2}{g^{(0)} + g^{(0)}_{12}}, \tag{1.20}$$

and the respective Bogoliubov spectra

$$E^2_+ = (1 + \delta_+\mu)\Big(\frac{2\mu}{1 + \delta_+\mu} + \epsilon_k\Big)\epsilon_k, \tag{1.21}$$

$$E^2_- = (1 + \delta_-\mu)\Big(\frac{2\lambda\mu}{1 + \delta_-\mu} + \epsilon_k\Big)\epsilon_k, \tag{1.22}$$

with

$$\delta_\pm = \frac{4m}{\hbar^2}\Big(\frac{g^{(2)} \pm g^{(2)}_{12}}{g^{(0)} + g^{(0)}_{12}}\Big), \qquad \lambda = \frac{g^{(0)} - g^{(0)}_{12}}{g^{(0)} + g^{(0)}_{12}}. \tag{1.23}$$

1.3 Three-dimensional model

It is well known from scattering theory that in three spatial dimensions the s-wave scattering length a and the s-wave effective range of interaction r are the coefficients of the following expansion of the phase shift $\delta(k)$ [93, 94]

$$k \cot[\delta(k)] = -\frac{1}{a} + \frac{1}{2} r k^2 + O(k^4) + ..., \tag{1.24}$$

where k^2 is the energy in units of $\hbar^2/2m$, and m is the reduced mass. In obtaining the couplings constants in Eq. (**??**), we briefly describe some general aspects related to their calculation in a recently perspective [95], and we also include extra elements in the appendix C. By adopting an on-shell approximation for the T-matrix equation, analytical expressions connecting the Fourier transform of the interaction potential to the s-wave phase shift are obtained. In particular, explicit forms of the low-momentum parameters in terms of the s-wave scattering length and the effective-range of the interactions are calculated. So the matrix element of the transition operator of scattering theory is decomposed into partial waves. The orthogonality of Legendre functions, and the uniqueness of the representation in partial waves are used. Likewise, it is chosen the term with $l = 0$ (with l the degree of Legendre polynomials) i.e. it is selected the s-wave term. Finally, the on-shell approximation is performed [93, 94, 95]. As a consequence, the matrix element or s-wave transition element takes the form

$$T_{l=0}(k) = V_{l=0}(k) + V_{l=0}(k) C(k) T_{l=0}(k), \tag{1.25}$$

with the Fourier transform of the spherically-symmetric interaction potential $V(k)$ and, the dimensional dependent constant $C(k)$. In $3d$ case we have

$$C(k) = -i \frac{m}{4\pi\hbar^2} k. \tag{1.26}$$

Moreover, the scattering theory shows that $T_{l=0}(k)$ is written in terms of the s-wave scattering amplitude $f_{l=0}(k)$ as follows

$$T_{l=0}(k) = -\frac{4\pi\hbar^2}{m} f_{l=0}(k). \tag{1.27}$$

In turn the s-wave scattering amplitude $f_{l=0}(k)$ is related to the s-wave phase shift $\delta_{l=0}(k)$ by means of

$$f_{l=0}(k) = \frac{1}{k[\cot[\delta(k)] - \mathrm{i}]}. \tag{1.28}$$

Thus, from Eqs. (1.25)-(1.28) we get,

$$V_{l=0}(k) = -\frac{4\pi\hbar^2}{m}\frac{\tan[\delta_{l=0}(k)]}{k}. \tag{1.29}$$

So by using the expansion given by Eq. (1.24) into Eq. (1.29), and taking into account the Taylor expansion of $V_{l=0}(k)$ with respect to k, such that, $V_{l=0}(k) = g^{(0)} + g^{(2)}k^2 + ...$, we obtain the following interacting $3d$ Bose-Bose intra-species (inter-species) coupling constants

$$g^{(0)} = \frac{4\pi\hbar^2}{m}a, \qquad g^{(0)}_{12} = \frac{4\pi\hbar^2}{m}a_{12}, \tag{1.30}$$

and

$$g^{(2)} = \frac{2\pi\hbar^2}{m}a^2 r, \qquad g^{(2)}_{12} = \frac{2\pi\hbar^2}{m}a^2_{12} r_{12}. \tag{1.31}$$

Expressions in Eq. (1.30) are well known for dilute and ultracold atomic gases. This kind of couplings arise when it is worthwhile replacing the two-body interaction potential between atoms with a pseudo-potential. The most usual, and simple, scheme consists in using the zero-range Fermi pseudo-potential. Nevertheless, an improvement of the previous contact or zero-range approximation can be achieved by replacing the interaction potential with a pseudo-potential [75, 83]. In such a case it is possible to obtain the expressions in Eq. (1.31).

It is remarkable to mention that applicability of expansion (1.24) holds under the condition $r \ll a$. In addition a physically reasonable assumption to an expansion for $r \gg a$ is given by [96]

$$\frac{1}{k}\tan[\delta(k)] = -a + \frac{1}{6}r^3 k^2 + ..., \tag{1.32}$$

which gives a good description of low-energy scattering processes. Instead Eq. (1.27) leads to the new nonuniversal couplings

$$g^{(2)} = -\frac{2\pi\hbar^2}{3m}r^3, \qquad g^{(2)}_{12} = -\frac{2\pi\hbar^2}{3m}r^3_{12}, \tag{1.33}$$

The coupling constants for zero-range interactions keep as in Eq. (1.30).

From the symmetric grand-potential in Eq. (1.20) and using the coupling for zero-range interactions in Eq. (1.30), the energy per particle in the mean-field approximation can be read as

$$\frac{E_0}{N} = \frac{1}{4}\Big(1 + \frac{a_{12}}{a}\Big) g^{(0)} n. \tag{1.34}$$

On the other hand, from Eq. (1.19), with $d = 3$, and performing dimensional regularization, as in appendix D, we obtain the grand-potential [51, 82]

$$\frac{\Omega_{\mathrm{GF}}}{L^3} = \frac{8}{15\pi^2}\Big(\frac{m}{\hbar^2}\Big)^{3/2} \frac{\mu^{5/2}}{(1+\delta_+\mu)^2} + \frac{8}{15\pi^2}\Big(\frac{m}{\hbar^2}\Big)^{3/2} \frac{\lambda^{5/2}\mu^{5/2}}{(1+\delta_-\mu)^2}. \tag{1.35}$$

From this grand potential we also obtain the Lee-Huang-Yang-like (LHY-like) correction to the energy per particle. Therefore the total energy per particle at zero-temperature of $3d$ Bose-Bose mixtures including nonuniversal corrections to the interactions can be read as

$$\begin{aligned} \frac{E_{NUC}}{N} &= (a + a_{12})\frac{\pi\hbar^2}{m} n + \frac{32\sqrt{2\pi}}{15}\frac{\hbar^2}{m}\frac{(a+a_{12})^{5/2} n^{3/2}}{\big[1 - \frac{4}{3}\pi(r^3 + r_{12}^3)n\big]^2} \\ &+ \frac{32\sqrt{2\pi}}{15}\frac{\hbar^2}{m}\frac{(a-a_{12})^{5/2} n^{3/2}}{\big[1 - \frac{4}{3}\pi(r^3 - r_{12}^3)n\big]^2}, \end{aligned} \tag{1.36}$$

we have choose the couplings given in Eq. (1.33). Instead for couplings in Eq. (1.31) we can use

$$r^3 \pm r_{12}^3 \to -3(a^2 r \pm a_{12}^2 r_{12}). \tag{1.37}$$

In absence of the nonuniversal effects of the interactions we recover the result obtained in Refs. [23], and [51], such that

$$\frac{E}{N} = (a + a_{12})\frac{\pi\hbar^2}{m} n + \frac{32\sqrt{2\pi}}{15}\frac{\hbar^2}{m}\big[(a+a_{12})^{5/2} + (a-a_{12})^{5/2}\big] n^{3/2}. \tag{1.38}$$

In presence or in absence of the nonuniversal corrections to the interactions we can see that for attractive inter-species interactions ($a_{12} < 0$) slightly larger than repulsive intra-species interactions ($a > 0$), such that, $|a_{12}|/|a| \sim -1^-$, the energy per particle becomes complex, rendering the mixture unstable [23]. However, if we consider the approximation $-a_{12} = a$ in the fluctuations only, as it was done by Petrov in Ref. [23], the energy per particle keeps real, and Eq. (1.38) reduces to the free droplet phase with energy per particle

$$\frac{E_D}{N} = -|a - a_{12}|\frac{\pi\hbar^2}{m}n + \frac{256\sqrt{\pi}}{15}\frac{\hbar^2}{m}a^{5/2}n^{3/2}. \tag{1.39}$$

It is worth mentioning that the term $(a + a_{12})^{5/2} + (a - a_{12})^{5/2}$ in the fluctuations contribution of Eq. (1.38) is symmetric under $a_{12} \to -a_{12}$. Therefore the same droplet can arise in another equivalent situation where $a_{12} = a$ in the fluctuations only [23, 47]. So providing that $a_{12} = a$ or $-a_{12} = a$ just in the Gaussian corrections to the total energy per particle in Eq. (1.36), the system exhibits a liquidlike phase where the $3d$ droplet with nonuniversal corrections to the interactions (DNUC) emerges with energy per particle

$$\frac{E^{\pm}_{DNUC}}{N} = -|a - a_{12}|\frac{\pi\hbar^2}{m}n + \frac{256\sqrt{\pi}}{15}\frac{\hbar^2}{m}\frac{a^{5/2}n^{3/2}}{\left[1 - \frac{4}{3}\pi(r^3 \pm r_{12}^3)n\right]^2}. \tag{1.40}$$

We use the couplings in Eq. (1.33) considering that in absence of the fluctuations the attractive effect of the interactions, such that $-a_{12} > a$, causes the condensate to collapse therefore the strong attraction lead us to consider the nonuniversal corrections to the attractive interactions such that $r_{12} \gg a_{12}$, as a relevant contribution. However we must keep in mind that although attraction is greater than repulsion, the repulsion is very close to the attraction and in turn such a repulsion encoded in a controls the fluctuations. In this sense, and in order to have a more complete overview of the effects of the nonuniversal corrections to the interactions we also include the nonuniversal correction to the repulsion such that $r \gg a$. Nevertheless neglecting the nonuniversal corrections to the repulsive interactions, and using the nonuniversal contribution of the attractive interactions as a fitting parameter we obtain a good agreement between our theoretical predictions and some diffusion Monte Carlo calculations (DMC) [47], as we will see later. Experimental values of the s-wave scattering length and the nonuniversal corrections to the interactions as a function of the external magnetic field in ultracold ^{39}K atoms show that it is possible to satisfy the condition $r \gg a$ [48, 97].

In Fig. 1.1 we plot the energy per particle given by Eqs. (1.36), and (1.38)-(1.40). We consider $\hbar^2/(2ma^2)$ as the energy unit, and we define $\gamma = r/a$, and $\gamma_{12} = r_{12}/a$. The energies are considered for an experimentally relevant density in the conventional droplet regime, $na^3 \sim 10^{-5}$ [25, 26]. We choose the negative sign for the DNUC in Eq. (1.40). We set $a < -a_{12}$ in the fluctuations of Eq. (1.36),

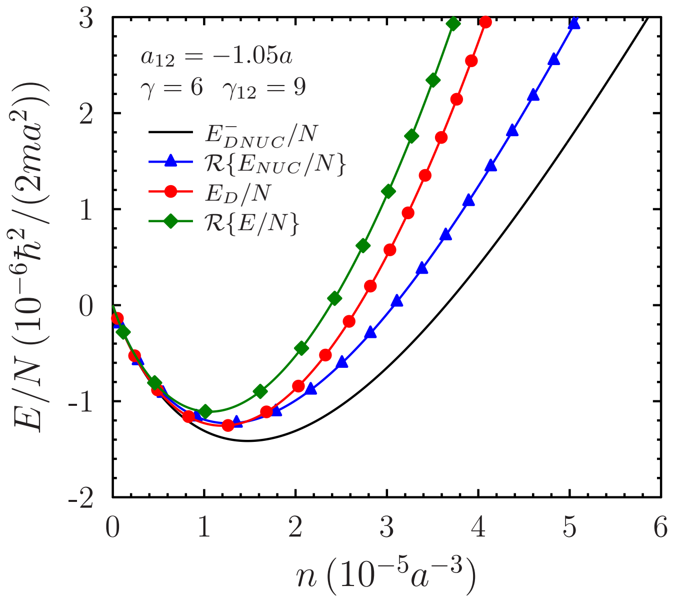

Figure 1.1: Three-dimensional energy per particle of Bose-Bose gases with nonuniversal corrections to the interactions as function of the density. We consider attractive interspecies interactions such that $a_{12} = -1.05a$. We use $\hbar^2/(2ma^2)$ as the energy unit, and we set $\gamma = r/a = 6$, and $\gamma_{12} = r_{12}/a = 9$. The energy per particle of droplets with nonuniversal corrections to the interactions E^{-}_{DNUC}/N is given by Eq. (1.40) (solid black line). The real contribution of Eq. (1.36) is $\mathcal{R}\{E_{NUC}/N\}$ with $a < -a_{12}$, (blue triangles). We also include the usual droplet given in Eq. (1.39), E_D/N, (red circles). Real contribution of Eq. (1.38), $\mathcal{R}\{E/N\}$, (green diamonds), is also included.

and $\mathcal{R}\{E_{NUC}/N\}$ corresponds to real part of (1.36). As a physically reasonable assumption we neglect the imaginary term providing $\mathcal{I}\{E_{NUC}/N\} \ll \mathcal{R}\{E_{NUC}/N\}$. In a similar way we have $\mathcal{R}\{E/N\}$ using Eq. (1.38). At very low densities $n \lesssim 5 \times 10^{-6}a^{-3}$ the nonuniversal contribution to the energy in Eqs. (1.36) and (1.40) could be neglected, reproducing the energies in Eqs. (1.38) and (1.39) respectively. In turn the energies in Eqs. (1.38) and (1.39) produce almost the same result, as it is expected. However, for values greater than this density we can see a clear difference between models predictions. For both the DNUC and the real contribution of the energy per particle including the nonuniversal effects of the interactions the density of particles is greater than their counterparts without the enhanced nonuniversal effects. This behavior can be understood in the following way, if $\gamma_{12}^3 - \gamma^3 > 0$ the nonuniversal correction to the attraction exceeds that of repulsion. Thus the effective contribution given by the nonuniversal effects to the interactions allows an increasing in the attraction which in turn allows that equilibrium density increases. For large values of $\gamma_{12}^3 - \gamma^3 > 0$ inelastic collisions decreases the number of atoms that can be accommodated in a self-

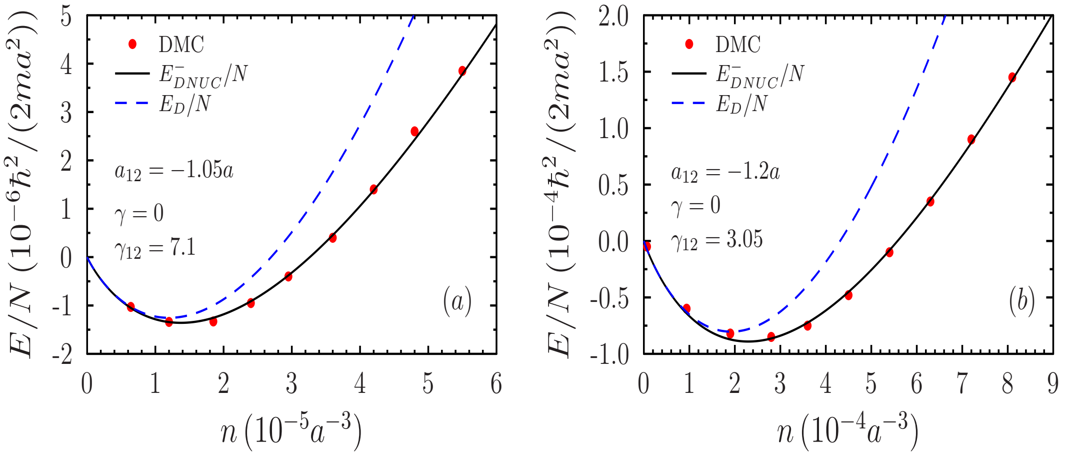

Figure 1.2: Three-dimensional energy per particle of Bose-Bose gases with nonuniversal corrections to the interactions as function of the density. The energy per particle of DNUC, E^-_{DNUC}/N is given by Eq. (1.40) (solid black line). The usual droplet given in Eq. (1.39), E_D/N, (dashed blue line). The diffusion Monte Carlo (DMC) results are given from [47] (red dots). We use $\hbar^2/(2ma^2)$ as the energy unit. (a) We set the attractive inter-species interactions such that $a_{12} = -1.05a$. The nonuniversal corrections for the repulsion and for the attraction are $\gamma = 0$ and $\gamma_{12} = 7.1$, respectively. (b) we consider $a_{12} = -1.2a$, $\gamma = 0$ and $\gamma_{12} = 3.05$.

bound state and we no longer find a minimum in the energy per particle. The DNUC undergoes instability and it disappears. There is not a stable self-bound state. Otherwise, when the nonuniversal correction to the repulsion exceeds that of attraction, holding the condition $\gamma_{12}^3 - \gamma^3 < 0$, the total effective repulsion causes decreasing in the number of atoms forming the DNUC. So the equilibrium density and the associated energy are lower than their counterparts without the nonuniversal effects. Using the couplings of Eq. (1.31) we have $\gamma, \gamma_{12} \ll 1$ and their effects on the energies per particle of Eqs. (1.36) and (1.40) are not perceptible. It is remarkable that the behavior presented in Fig. 1.1 is similar to one obtained for usual droplets in numerical calculations [46, 47, 48].

In Fig. 1.2 we compare the energy per particle of DNUC, given by Eq. (1.40) with some DMC results given in [47]. We consider two different attractive inter-species interactions such that $a_{12} = -1.05a$, and $a_{12} = -1.2a$. Taking into account that the attraction is leading we set the nonuniversal effects to the repulsive interactions as $\gamma = 0$. The nonuniversal effects to the attractive interactions are chosen as fitting parameters with $\gamma_{12} = 7.1$ and $\gamma_{12} = 3.05$. We also include the energy per particle for the usual droplet given in Eq. (1.39). In particular the minimum energy n_0 predicted by Eq. (1.39) is ~ 1.198, and by means of Eq. (1.40) we found ~ 1.476, so we have $n_{0,DNUC} \sim 1.232 n_{0,D}$. We can also see that if $a \sim$

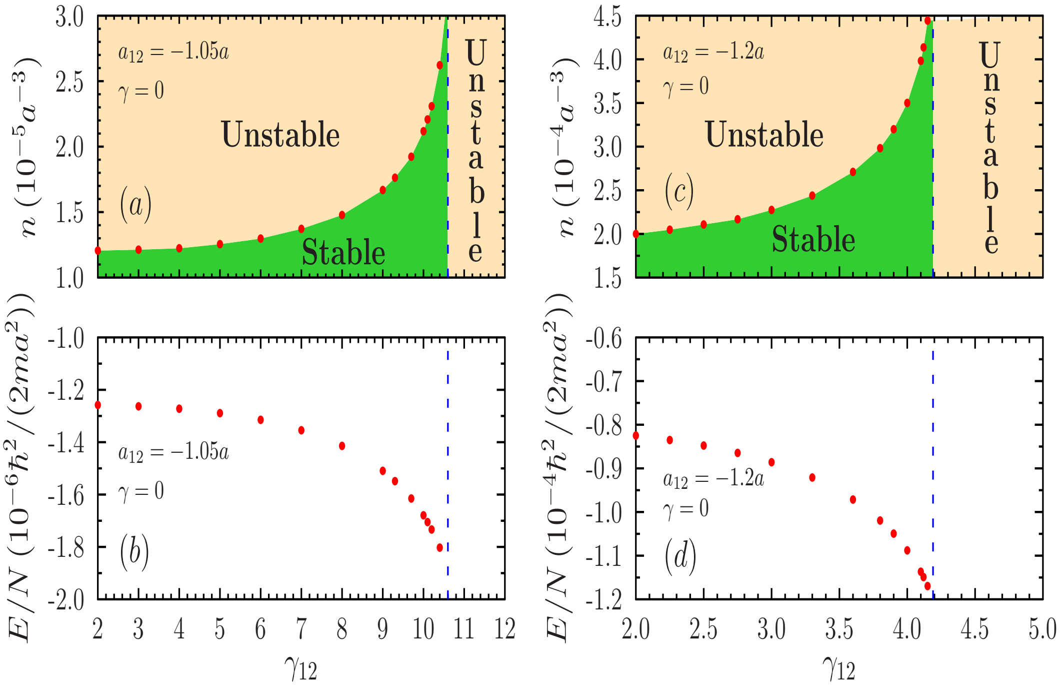

Figure 1.3: Phase diagram and energy per particle for DNUC as function of the nonuniversal effects of the attractive interactions γ_{12}. The red dots are obtained from Eq. (1.40) as the minimum density or minimum energy per particle for a stable DNUC formation. The nonuniversal correction to the repulsion is fixed as $\gamma = 0$. We use $\hbar^2/(2ma^2)$ as the energy unit.(a)-(b) we set the attractive inter-species interactions such that $a_{12} = -1.05a$. (c)-(d) we consider $a_{12} = -1.2a$. The dashed blue line represents the threshold value for γ_{12}.

100Å we obtain densities with experimental relevance. Thus $n \sim 10^{13}$atoms/cm^3 and $n \sim 10^{14}$atoms/cm^3 in Fig. 1.2(a) and Fig. 1.2(b) respectively.

By using Eq. (1.40) we plot the phase diagram and energy per particle for DNUC as function of the nonuniversal effects of the attractive interactions γ_{12} in Fig. 1.3. The nonuniversal correction to the repulsion is fixed as $\gamma = 0$. We use $\hbar^2/(2ma^2)$ as the energy unit. In Fig. 1.3(a)-(b) we set the attractive inter-species interactions such that $a_{12} = -1.05a$. In Fig. 1.3(c)-(d) we consider $a_{12} = -1.2a$. The blue line represents the threshold values of γ_{12} with $\gamma_{12} \sim 10.6$ and $\gamma_{12} \sim 4.19$, for $a_{12} = -1.05a$, and $a_{12} = -1.2a$, respectively. In Fig. 1.3 we show how increasing the nonuniversal correction to the attractions, the density increases, the DNUC is more attractive and eventually this becomes unstable, as it was explained above. We can also see how the threshold for the instability is smaller as the attractive scattering length increases, as it is expected. This can be understood due to the fact that the leading contribution is attractive. In Fig. 1.4 we also plot the phase diagram and energy per particle for DNUC as function of the dimensionless attractive scattering length a_{12}/a with fixed values of γ and γ_{12}. This behavior is

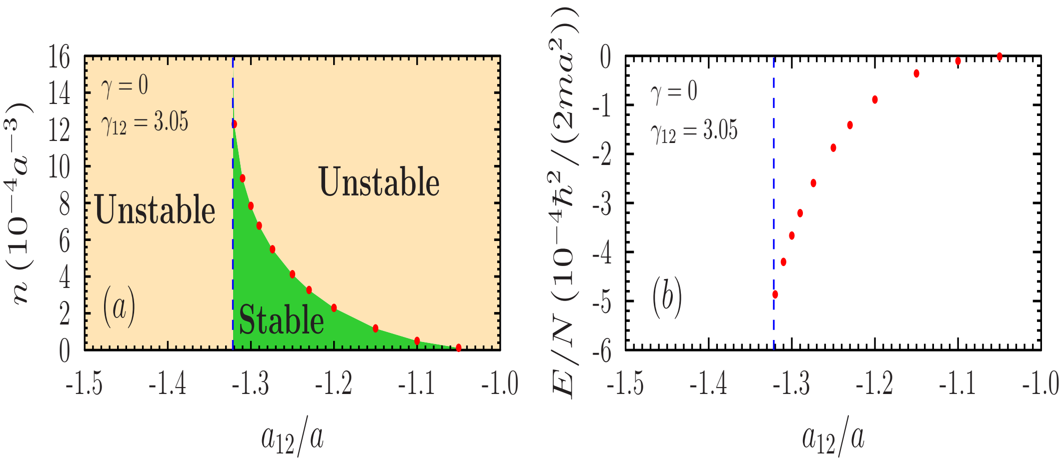

Figure 1.4: Phase diagram and energy per particle for DNUC as function of the dimensionless attractive scattering length a_{12}/a. The red dots are obtained from Eq. (1.40) as the minimum density or minimum energy per particle for a stable DNUC formation. The nonuniversal correction for the repulsion is fixed as $\gamma = 0$. We use $\hbar^2/(2ma^2)$ as the energy unit. We set the nonuniversal correction to the attractions as $\gamma_{12} = 3.05$. The dashed blue line represents the threshold value for a_{12}/a.

equivalent to that presented in the Fig. 1.3 and it is an obvious consequence of the DNUC instability when the leading contribution, the attraction, increases. In other words for values greater than $a_{12}/a \sim -1.3217$ the DNUC collapses.

Now, we present an improved $3d$ Gross-Pitaevskii equation (GPE) to describe the phase of droplets with nonuniversal corrections to the interactions in free space

$$\begin{aligned} i\hbar\frac{\partial\phi}{\partial t} &= \Big[-\frac{\hbar^2}{2m}\nabla^2 - \frac{2\pi\hbar^2}{m}|a_{12}-a||\phi|^2 + \frac{\pi\hbar^2}{3m}(r^3+r_{12}^3)\nabla^2|\phi|^2 \\ &+ \frac{128\sqrt{\pi}}{3}\frac{\hbar^2}{m}a|\phi|^2\sqrt{|\phi|^2a^3}F^{\pm}(r,r_{12},|\phi|^2)\Big]\phi, \end{aligned} \tag{1.41}$$

where

$$F^{\pm}(r,r_{12},|\phi|^2) = \frac{1-\frac{4\pi}{15}(r^3\pm r_{12}^3)|\phi|^2}{\left[1-\frac{4\pi}{3}(r^3\pm r_{12}^3)|\phi|^2\right]^3}. \tag{1.42}$$

The first two terms correspond to the usual attractive mean-field approximation in Bose-Bose gases. The third term describes the nonuniversal corrections to the interactions at level of mean-field approximation. The last contribution takes into account improved fluctuation effects including the nonuniversal corrections to the interactions where it was used $a = \pm a_{12}$. By increasing the density could be possible to find an instability associated to $F^{\pm}$, for both $a \gg r$ and $a \ll r$.

For $a \ll r$ the instability is present for $|\phi|^2 = 3/[4\pi(r^3 \pm r_{12}^3)]$, with $r > r_{12}$ choosing the negative sign. For $a \gg r$ the DNUC becomes unstable for $|\phi|^2 = 1/[4\pi(a_{12}^2 r_{12} - a^2 r)]$, with $a_{12}^2 r_{12} > a^2 r$. Since $r^3 + r_{12}^3 > 0$, the nonuniversal corrections to the interactions are repulsive at mean-field level. At first glance, this would allow controlling the number of atoms into the self-bound liquidlike state. Increasing the strength of the repulsion beyond a critical value the atoms could be spreading out decreasing on the number of atoms necessary to obtain a stable DNUC. This could be helpful for fitting with experimental or numerical evidence. It is also remarkable and interesting to consider only the mean-field approximation, without fluctuations. The attraction-repulsion balance could allow a few atoms to be accommodated into a stable bound-state formation, but not including Gaussian corrections. Although the nonuniversal corrections to the interactions are not leading, these could in principle play a similar role as the LHY contribution in a conventional droplet. In a different scenario this equation could be useful to study how solitons and vortices are affected by such a nonuniversal corrections to the interactions. Finally, taking into account the improved GPE with the change given by Eq. (1.37) it could be interesting even in a context other than droplets.

1.3.1 Three-dimensional finite-temperature effects

We briefly describe some aspects regarding finite-temperature corrections to the equation of state of $3d$ Bose-Bose mixtures with nonuniversal corrections to the interactions. In the continuum limit the $3d$ one-loop correction to the grand potential in Eq. (1.18) is written as [51],

$$\frac{\Omega_{\mathrm{GF}}^{(T)}}{L^3} = -\frac{1}{6\pi^2}\sum_{\pm}\int_0^{\infty} dE_{\pm}(k_{\pm})\frac{k_{\pm}^3}{e^{\beta E_{\pm}(k)}-1}, \tag{1.43}$$

and Bogoliubov spectra in Eq. (1.21) lead to

$$k_{+}^2 = \frac{2m}{\hbar^2}\frac{\mu}{1+\delta_{+}\mu}\left(\sqrt{1+\frac{(1+\delta_{+}\mu)}{\mu^2}E_{+}^2}-1\right), \tag{1.44}$$

and

$$k_{-}^2 = \frac{2m}{\hbar^2}\frac{\lambda\mu}{1+\delta_{-}\mu}\left(\sqrt{1+\frac{(1+\delta_{-}\mu)}{\lambda^2\mu^2}E_{-}^2}-1\right), \tag{1.45}$$

with $\delta_\pm$, and λ given in Eq. (1.23). Now, after introducing the variables $x_\pm = \beta E_\pm$, and expanding $k_\pm$ at low temperature $k_B T \ll |\mu|$ [44, 45], we get

$$\begin{aligned}\frac{\Omega^{(T)}_{\rm GF}}{L^3} &= -\frac{\pi^2}{90}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{(k_BT)^4}{\mu^{3/2}}\left[1-\frac{5\pi^2}{7}\frac{(1+\delta_+\mu)}{\mu^2}(k_BT)^2\right] \\ &- \frac{\pi^2}{90}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{(k_BT)^4}{\lambda^{3/2}\mu^{3/2}}\left[1-\frac{5\pi^2}{7}\frac{(1+\delta_-\mu)}{\lambda^2\mu^2}(k_BT)^2\right]. \end{aligned} \tag{1.46}$$

From which it follows the thermal energy per particle

$$\begin{aligned}\frac{E^{(T)}_{\rm GF}}{N} &= \frac{\sqrt{2\pi}}{240}\left(\frac{m}{\hbar^2}\right)^{3}\frac{(k_BT)^4}{(a+a_{12})^{3/2}n^{5/2}}(1+h^+_{NUC}) \\ &+ \frac{\sqrt{2\pi}}{240}\left(\frac{m}{\hbar^2}\right)^{3}\frac{(k_BT)^4}{(a-a_{12})^{3/2}n^{5/2}}(1+h^-_{NUC}), \end{aligned} \tag{1.47}$$

with

$$h^\pm_{NUC} = -\frac{5}{84}\left(\frac{m}{\hbar^2}\right)^2\frac{(k_BT)^2}{(a\pm a_{12})^2n^2}\left[3-\frac{20\pi}{3}(r^3\pm r^3_{12})n\right], \tag{1.48}$$

where we used the coupling constants from expression (1.33). It is remarkable that unlike the zero-temperature corrections the above thermal improvement is divergent provided $a = \pm a_{12}$ and the mixture undergoes a thermally instability. In a similar way for attractive interspecies interactions lightly larger than repulsive intra-species interaction, Eq. (1.47) becomes complex for both DNUC and usual droplets ($r = r_{12} = 0$). However, compared to corrections in Eq. (1.36), in this case the imaginary contribution is leading. Therefore both the DNUC and the usual droplets are thermal-induced unstables. We also highlight that the nonuniversal corrections appear only up at order T^6 and, hence at very low temperatures these could be neglected.

1.4 Two-dimensional model

We focus on two-dimensional Bose-Bose gases. Two-dimensional scattering theory indicates that the expansion of the phase shift $\delta_{l=0}(k)$, can be read as [98]

$$\cot[\delta(k)] = \frac{2}{\pi}\ln\left(\frac{k}{2}ae^\gamma\right) + \frac{1}{2}rk^2 + ..., \tag{1.49}$$

with the s-wave scattering length a, the s-wave effective range of interaction r, the condition $a \gg r$, and $\gamma = 0.5572...$ the Euler-Mascheroni constant. The $2d$ coefficient $C(k)$ in the s-wave transition element given in Eq. (1.25) is written as [95], see appendix C

$$C(k) = \frac{m}{2\pi\hbar^2} \ln\left(\frac{k}{\sqrt{\epsilon_c}}\right) - \frac{m}{4\hbar^2}\mathrm{i}, \tag{1.50}$$

with the low-energy cutoff $\epsilon_c = \hbar^2\bar{\kappa}^2/m$. In $2d$ scattering theory the s-wave phase shift $\delta(k)$ and the s-wave transition element $T_{l=0}(k)$ are related by means of [99]

$$T_{l=0}(k) = -\frac{4\pi\hbar^2}{m}\frac{1}{\cot[\delta_{l=0}(k)] - \mathrm{i}}. \tag{1.51}$$

So, inserting Eq. (C.11) into Eq. (1.25), and comparing with (1.51) we get,

$$V_{l=0}(k) = -\frac{4\pi\hbar^2}{m}\frac{1}{\cot[\delta_{l=0}(k)] - \frac{2}{\pi}\ln\left(\frac{k}{\sqrt{\epsilon_c}}\right)}. \tag{1.52}$$

Inserting Eq. (1.49) into Eq. (1.52) and taking into account the Taylor expansion at low momentum of $V_{l=0}(k)$ where $V_{l=0}(k) = g^{(0)} + g^{(2)}k^2 + ...$, we can obtain the $2d$ intra-species interacting coupling constants

$$g^{(0)} = \frac{4\pi\hbar^2}{m}\frac{1}{\ln\left(\frac{4e^{-2\gamma}}{a^2\epsilon_c}\right)}, \tag{1.53}$$

and

$$g^{(2)} = -\frac{2\pi^2\hbar^2}{m}\frac{r^2}{\ln^2\left(\frac{4e^{-2\gamma}}{a^2\epsilon_c}\right)}. \tag{1.54}$$

In a similar way the inter-species coupling constants are

$$g_{12}^{(0)} = \frac{4\pi\hbar^2}{m}\frac{1}{\ln\left(\frac{4e^{-2\gamma}}{a_{12}^2\epsilon_c}\right)}, \tag{1.55}$$

and,

$$g_{12}^{(2)} = -\frac{2\pi^2\hbar^2}{m}\frac{r_{12}^2}{\ln^2\left(\frac{4e^{-2\gamma}}{a_{12}^2\epsilon_c}\right)}. \tag{1.56}$$

From symmetric grand-potential in Eq. (1.20) and the coupling constants of zero-range interactions in Eqs. (1.53) and (1.55), the $2d$ mean-field energy per particle is given by

$$\frac{E}{N} = \frac{1}{4}\Big(1 + \frac{g_{12}^{(0)}}{g^{(0)}}\Big) g^{(0)} n. \tag{1.57}$$

In Eq. (1.19) with $d = 2$ and performing dimensional regularization in the modified minimal subtraction scheme $\overline{\text{MS}}$-scheme [55], see also appendix D, leads us to the following grand-potential including nonuniversal corrections to the interactions

$$\begin{aligned} \frac{\Omega_{\text{GF}}}{L^2} &= -\frac{m}{8\pi\hbar^2} \frac{\mu^2}{(1+\delta_+\mu)^{3/2}} \ln\Big[\frac{\epsilon_c}{\sqrt{e}} \frac{(1+\delta_+\mu)}{\mu}\Big] \\ &- \frac{m}{8\pi\hbar^2} \frac{\lambda^2\mu^2}{(1+\delta_-\mu)^{3/2}} \ln\Big[\frac{\epsilon_c}{\sqrt{e}} \frac{(1+\delta_-\mu)}{\lambda\mu}\Big]. \end{aligned} \tag{1.58}$$

The $2d$ energy per particle of Bose-Bose mixtures could be obtained through the conventional thermodynamic relations in the grand-canonical ensemble. However we are interested and we will focus on the case of weakly attractive inter- and weakly repulsive intra-species interactions, where $a_{12}^{-1} \ll \sqrt{n} \ll a^{-1}$ [24, 55]. For simplicity, we set $m = \hbar = 1$. In order to obtain the energy per particle in this regime we introduce a new energy cutoff $\tilde{\epsilon}_c$, such that, $\tilde{\epsilon}_c = 4e^{-2\gamma}/(aa_{12})$ [24, 55]. Provided that $\tilde{\epsilon}_c/\epsilon_c$ is not exponentially large we can use $\epsilon_c \to \tilde{\epsilon}_c$ as a good assumption from which we get the following coupling constants

$$g^{(0)} = \frac{4\pi}{\ln(a_{12}/a)}, \qquad g_{12}^{(0)} = \frac{4\pi}{\ln(a/a_{12})}, \tag{1.59}$$

where $g^{(0)} = -g_{12}^{(0)}$. In a similar way, the coupling constants with nonuniversal corrections to the interactions are

$$g^{(2)} = -\frac{2\pi^2 r^2}{\ln^2(a_{12}/a)}, \qquad g_{12}^{(2)} = -\frac{2\pi^2 r_{12}^2}{\ln^2(a_{12}/a)}, \tag{1.60}$$

where $g_{12}^{(2)}/g^{(2)} = (r_{12}/r)^2$. So we get the energy per particle of $2d$ DNUC as

$$\begin{aligned} \frac{E_{DNUC}}{N} &= \frac{1}{8\pi} \frac{[g^{(0)}]^2 n}{\big[1 + 2g^{(2)}\big[1 - (\frac{r_{12}}{r})^2\big] n\big]^{3/2}} \\ &\times \ \ln\Big[\frac{e^{2\gamma+1/2}}{4} \frac{a a_{12} g^{(0)} n}{1 + 2g^{(2)}\big[1 - \big(\frac{r_{12}}{r}\big)^2\big] n}\Big]. \end{aligned} \tag{1.61}$$

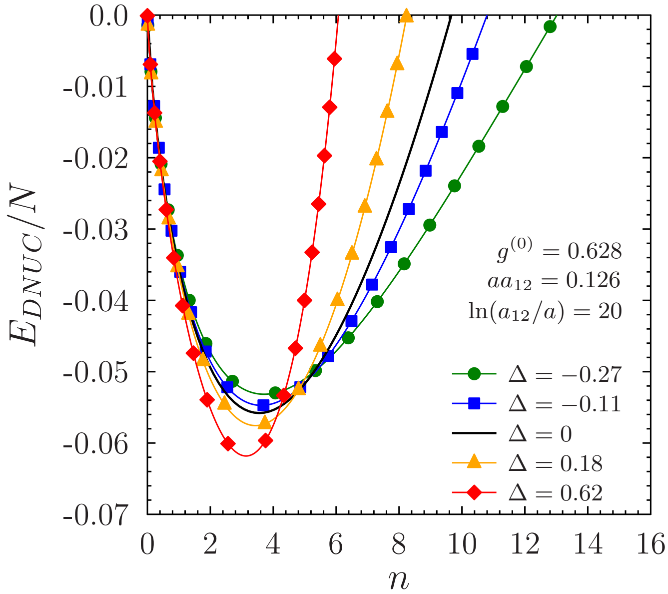

Figure 1.5: Two-dimensional energy per particle of droplets with nonuniversal corrections to the interactions as function of the density, Eq. (1.64). We fix $g^{(0)} = 0.628$, $aa_{12} = 0.126$ and $\ln(a_{12}/a) = 20$, and we define $\Delta \equiv 1 - (r_{12}/r)^2$. We include $\Delta = -0.27$ (green circles), $\Delta = -0.11$ (blue squares), $\Delta = 0.18$ (orange triangles) and $\Delta = 0.62$ (red diamonds). $\Delta = 0$ (solid black line) corresponds to absence of nonuniversal improvements to the interactions given in Ref. [24].

In absence of the nonuniversal effects to the interactions or in the symmetric case $r = r_{12}$, the energy per particle in Eq. 1.61 describes the conventional 2d droplet phase [24], where

$$\frac{E}{N} = \frac{2\pi n}{\ln^2(a_{12}/a)} \ln\left(\frac{n}{en_0}\right), \tag{1.62}$$

with n_0 the equilibrium density

$$n_0 = \frac{1}{\pi} e^{-2\gamma - 3/2} \frac{\ln(a_{12}/a)}{aa_{12}}. \tag{1.63}$$

From Eqs. (1.62) and (1.63) we can write Eq. (1.61) as

$$\frac{E_{DNUC}}{N} = \frac{2\pi\, n}{\ln^2(a_{12}/a)} \frac{1}{h_{NUC}^{3/2}} \ln\left(\frac{n}{en_0}\frac{1}{h_{NUC}}\right), \tag{1.64}$$

with $h_{NUC} = 1 + f_{NUC}|\phi|^2$, and $f_{NUC} = 2g^{(2)}[1 - (r_{12}/r)^2]$.

In Fig. 1.5 we plot the energy per particle from Eq. (1.64) as density function. We set the values $g^{(0)} = 0.628$, $aa_{12} = 0.126$ and $\ln(a_{12}/a) = 20$. We define $\Delta \equiv$

$1-(r_{12}/r)^2$, and we consider different values and change of sign for this parameter. The case $\Delta = 0$ corresponds to results in absence of nonuniversal corrections to the interactions obtained in Ref. [24]. For $\Delta < 0$ the nonuniversal correction to the attraction exceeds that of repulsion. However the equilibrium density is only slightly larger than in absence of nonuniversal effects to the interactions. If nonuniversal correction to the repulsion exceeds that of attraction, it holds the condition $\Delta > 0$, and the equilibrium density is only slightly lower than in absence of nonuniversal effects of the interactions. A possible explanation for not observing significant changes could be associated with the use of coupling constants. In such a case we consider $a \gg r$, but taking into account the perturbative nature of the self-bound liquidlike phase could be suitable consider coupling constants associated to $a \ll r$.

Now, we introduce the improved $2d$ GPE to describe free DNUC

$$\begin{aligned} \mathrm{i}\frac{\partial\phi}{\partial t} &= \Big[-\frac{1}{2}\nabla^2 + \frac{2\pi^2}{\ln^2(a_{12}/a)}(r^2+r_{12}^2)\nabla^2|\phi|^2 \\ &+ \frac{4\pi}{\ln^2(a_{12}/a)}\frac{|\phi|^2}{h_{NUC}^{5/2}}\Big[\big(1+\frac{1}{4}f_{NUC}|\phi|^2\big)\ln\Big(\frac{|\phi|^2}{en_0}\frac{1}{h_{NUC}}\Big)+\frac{1}{2}\Big]\Big]\phi, \end{aligned} \tag{1.65}$$

where n_0 is given in Eq. (1.63). The first line corresponds to the mean-field approximation. The second line corresponds to the fluctuations including the nonuniversal corrections to the interactions. At first glance, given Eq. (1.59), the coupling of the nonuniversal corrections to the interactions provides a repulsive contribution at the mean-field level in Eq. (1.65). However, the dynamics of this $2d$ improved GPE is much more complex. We are including the dependence on the nonuniversal contribution to the interactions to the already known logarithmic dependence. In particular, under the physically reasonable assumption which nonuniversal contributions to the interactions are neglected in the fluctuation sector a simplified version of the previous $2d$ improved GPE is read as

$$\begin{aligned} \mathrm{i}\frac{\partial\phi}{\partial t} &= \Big[-\frac{1}{2}\nabla^2 + \frac{2\pi^2}{\ln^2(a_{12}/a)}(r^2+r_{12}^2)\nabla^2|\phi|^2 \\ &+ \frac{4\pi}{\ln^2(a_{12}/a)}|\phi|^2\ln\big(\frac{|\phi|^2}{\sqrt{e}n_0}\big)\Big]\phi, \end{aligned} \tag{1.66}$$

This improved GPE exhibits a competition between subleading nonuniversal corrections to the interactions at mean-field level and Gaussian fluctuations associated to the zero-range approximation in the interaction potential. By means of this GPE it is possible to study how conventional $2d$ droplets and vortex droplets [100] are affected by the nonuniversal corrections to the interatomic interactions.

1.4.1 Two-dimensional finite-temperature effects

In the continuum limit the $2d$ one-loop correction to the grand potential in Eq. (1.18), is written as

$$\frac{\Omega^{(T)}_{\rm GF}}{L^2} = -\frac{1}{4\pi}\sum_{\pm}\int_0^{\infty} dE_{\pm}(k_{\pm})\frac{k^2_{\pm}}{e^{\beta E_{\pm}(k)}-1}, \tag{1.67}$$

with $k^2_{\pm}$ given by Eqs. (1.44) and (1.45). Now, after introducing the variables $x_{\pm} = \beta E_{\pm}$, and expanding $k_{\pm}$ at low temperature $k_B T \ll |\mu|$ [44, 45], it follows the $2d$ grand-canonical potential

$$\begin{aligned}\frac{\Omega^{(T)}_{\rm GF}}{L^2} &= -\frac{1}{4\pi}\Gamma(3)\zeta(3)\left(\frac{m}{\hbar^2}\right)\frac{(k_BT)^3}{\mu}\left[1-\frac{\Gamma(5)\zeta(5)}{4\Gamma(3)\zeta(3)}\frac{(1+\delta_+\mu)}{\mu^2}(k_BT)^2\right] \\ &- \frac{1}{4\pi}\Gamma(3)\zeta(3)\left(\frac{m}{\hbar^2}\right)\frac{(k_BT)^3}{\lambda\mu}\left[1-\frac{\Gamma(5)\zeta(5)}{4\Gamma(3)\zeta(3)}\frac{(1+\delta_-\mu)}{\lambda^2\mu^2}(k_BT)^2\right],\end{aligned} \tag{1.68}$$

with the Euler's gamma function $\Gamma(x)$ and the Riemann's zeta function $\zeta(x)$ [101]. Thus we get the respective thermal energy per particle as

$$\begin{aligned}\frac{E^{(T)}_{\rm GF}}{N} &= \frac{\Gamma(3)\zeta(3)}{2\pi}\left(\frac{m}{\hbar^2}\right)\frac{(k_BT)^3}{[g^{(0)}+g^{(0)}_{12}]n^2}\left[1-\frac{\Gamma(5)\zeta(5)}{\Gamma(3)\zeta(3)}\frac{(k_BT)^2}{[g^{(0)}+g^{(0)}_{12}]^2n^2}h^{+}_{NUC}\right] \\ &+ \frac{\Gamma(3)\zeta(3)}{2\pi}\left(\frac{m}{\hbar^2}\right)\frac{(k_BT)^3}{[g^{(0)}-g^{(0)}_{12}]n^2}\left[1-\frac{\Gamma(5)\zeta(5)}{\Gamma(3)\zeta(3)}\frac{(k_BT)^2}{[g^{(0)}-g^{(0)}_{12}]^2n^2}h^{-}_{NUC}\right],\end{aligned} \tag{1.69}$$

with

$$h^{\pm}_{NUC} = 1 + \frac{4m}{\hbar^2}[g^{(2)} \pm g^{(2)}_{12}]n. \tag{1.70}$$

Like in the $3d$ case, the above thermal improvements are divergent provided $a = \pm a_{12}$ and the Bose-Bose mixture exhibits a thermal instability. For attractive inter-species interactions lightly larger than repulsive intra-species interaction, the energy per particle becomes complex with leading imaginary contribution. Therefore both the $2d$ DNUC and the usual $2d$ droplets undergo thermal-induced instability. We also highlight that the effective nonuniversal corrections to the interactions appear only up at order T^5 and, hence at very low temperatures these could be neglected.

1.5 One-dimensional model

In one-dimensional scattering theory the expansion of the phase shift $\delta(k)$ is given by [102, 103]

$$k\tan[\delta(k)] = \frac{1}{a} + \frac{1}{2}rk^2 + ..., \tag{1.71}$$

with the s-wave scattering length a, the s-wave effective range of interaction r, and the condition $a \gg r$. The $1d$ coefficient $C(k)$ in the s-wave transition element given in Eq. (1.25) is written as [95], see appendix C

$$C(k) = -\frac{\mathrm{i}}{k}\frac{m}{2\hbar^2}. \tag{1.72}$$

In one-dimensional scattering theory the s-wave phase shift $\delta_{l=0}(k)$ and the s-wave transition element $T_{l=0}(k)$ are related by means of [102, 103]

$$T_{l=0}(k) = -\frac{2\hbar^2}{m}\frac{1}{\cot[\delta_{l=0}(k)] - \mathrm{i}}. \tag{1.73}$$

So, inserting Eq. (1.72) into Eq. (1.25), and comparing with (1.73) we get,

$$V_{l=0}(k) = -\frac{2\hbar^2}{m}k\tan[\delta_{l=0}(k)]. \tag{1.74}$$

Inserting Eq. (1.71) into Eq. (1.74) and taking into account the Taylor expansion at low momentum of $V_{l=0}(k)$ where $V_{l=0}(k) = g^{(0)} + g^{(2)}k^2 + ...$, we can obtain the $1d$ intra-species interacting coupling constants

$$g^{(0)} = -\frac{2\hbar^2}{ma}, \qquad g^{(2)} = -\frac{\hbar^2}{m}r. \tag{1.75}$$

In a similar way the inter-species coupling constants are

$$g_{12}^{(0)} = -\frac{2\hbar^2}{ma_{12}}, \qquad g_{12}^{(2)} = -\frac{\hbar^2}{m}r_{12}. \tag{1.76}$$

From the mean-field grand-potential in Eq. (1.20) and using the coupling constants in the zero-range approximation to the interactions in Eqs. (1.75) and (1.76), the energy per particle is given as

$$\frac{E_0}{N} = \frac{1}{4}\Big(1 + \frac{a}{a_{12}}\Big)g^{(0)}n. \tag{1.77}$$

From Eq. (1.19) with $d = 1$, and performing dimensional regularization, see appendix D, the grand-potential is given by [51, 82]

$$\frac{\Omega_{\mathrm{GF}}}{L} = -\frac{2}{3\pi}\Big(\frac{m}{\hbar^2}\Big)^{1/2}\frac{\mu^{3/2}}{1+\delta_+\mu} - \frac{2}{3\pi}\Big(\frac{m}{\hbar^2}\Big)^{1/2}\frac{\lambda^{3/2}\mu^{3/2}}{1+\delta_-\mu}. \tag{1.78}$$

So the $1d$ total energy per particle including the effects of the nonuniversal corrections to the interactions can be read as

$$\begin{aligned}\frac{E_{NUC}}{N} &= \frac{1}{4}(g^{(0)} + g_{12}^{(0)})n \\ &- \frac{1}{3\sqrt{2}\pi}\Big(\frac{m}{\hbar^2}\Big)^{1/2}\frac{[g^{(0)} + g_{12}^{(0)}]^{3/2}}{1+\frac{2m}{\hbar^2}(g^{(2)} + g_{12}^{(2)})n}n^{1/2} \\ &- \frac{1}{3\sqrt{2}\pi}\Big(\frac{m}{\hbar^2}\Big)^{1/2}\frac{[g^{(0)} - g_{12}^{(0)}]^{3/2}}{1+\frac{2m}{\hbar^2}(g^{(2)} - g_{12}^{(2)})n}n^{1/2}. \end{aligned} \tag{1.79}$$

As is known the stable formation of a droplet requires a subtle equilibrium between attraction and repulsion [23, 24]. In Eq. (1.79) we can see that such a balance is achieved providing $g^{(0)} + g_{12}^{(0)} > 0$ and $g^{(0)} > g_{12}^{(0)}$, and the liquidlike phase remains stable throughout. The first condition indicates that the mean-field energy per particle is repulsive and stable. The LHY-like corrections including the nonuniversal effects of the interactions are negative and these provide the necessary attractive contribution. Moreover due to the second condition, the LHY-like correction does not undergo from the issue of imaginary contributions, unlike the $3d$ model. Therefore we can use the full expression for the energy per particle without any approach that requires removal any of terms. Taking into account the above two mentioned conditions for a mixture with $g^{(0)} > 0$ and $g_{12}^{(0)} > 0$ the leading contribution is very repulsive and the attractive subleading contribution is not enough to allow the accommodation of a large number of atoms. Therefore predicted energies per particle are around two orders of magnitude smaller than those we will discuss in the following. Another way to obtain a

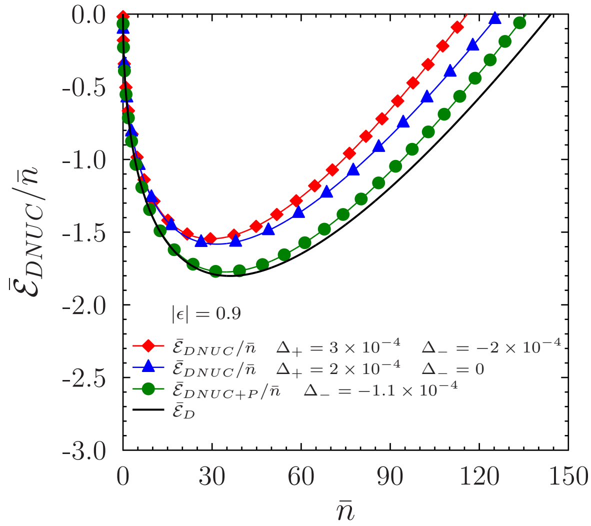

Figure 1.6: One-dimensional energy per particle of droplets with nonuniversal corrections to the interactions as function of the density, Eq. (1.80). We set $|\epsilon| = 0.9$, and define $\Delta_{\pm} = \bar{r} \pm \bar{r}_{12}$. We consider $\Delta_+ = 3 \times 10^{-4}$ and $\Delta_- = -2 \times 10^{-4}$ (red diamonds). $\Delta_+ = 2 \times 10^{-4}$ and $\Delta_- = 0$ (blue triangles). In the simplified version of Eq. (1.80) given by Eq. (1.81) we consider $\Delta_+ = -1.1 \times 10^{-4}$ (green circles). We also include results in absence of nonuniversal contributions to the interactions in Eq. (1.81) $\mathcal{E}_D$ (solid black line), given in Ref. [24].

balanced repulsion-attraction effect which leads to the emergence of a stable 1d DNUC or an usual droplet with higher energies per particle, consisting of using $|g^{(0)}| > |g_{12}^{(0)}|$ with $g^{(0)} > 0$, and $g_{12}^{(0)} < 0$, which corresponds to repulsive intra-species and attractive inter-species interactions, respectively. We focus on this last case. We use $g = 2\hbar^2/m|a|$, and $g_{12} = -2\hbar^2/m|a_{12}|$. We take $E_B = \hbar^2/m|a|^2$ as energy unit, we define $\epsilon = g_{12}^{(0)}/g^{(0)} < 0$, $\bar{n} = n|a|$, $\bar{r} = r/|a|$, $\bar{r}_{12} = r_{12}/|a|$, and $\bar{\mathcal{E}} = E/(LE_B/|a|)$. Thus these new variables lead to the scaled energy per particle of an uniform droplet with nonuniversal corrections to the interactions $\bar{\mathcal{E}}_{DNUC}/\bar{n}$ as

$$\begin{aligned}\frac{\bar{\mathcal{E}}_{DNUC}}{\bar{n}} &= \frac{1}{2}(1-|\epsilon|)\bar{n} - \frac{2}{3\pi}\sqrt{\bar{n}}\Big[\frac{(1-|\epsilon|)^{3/2}}{1-2(\bar{r}+\bar{r}_{12})\bar{n}} \\ &+ \frac{(1+|\epsilon|)^{3/2}}{1-2(\bar{r}-\bar{r}_{12})\bar{n}}\Big].\end{aligned} \tag{1.80}$$

Within Petrov's approximation, $|\epsilon| = 1$ only in the fluctuations, we have

$$\frac{\bar{\mathcal{E}}_{DNUC+P}}{\bar{n}} = \frac{1}{2}(1-|\epsilon|)\bar{n} - \frac{4\sqrt{2}}{3\pi}\frac{\sqrt{\bar{n}}}{1-2(\bar{r}-\bar{r}_{12})\bar{n}}. \tag{1.81}$$

In Fig 1.6, we plot Eq. (1.80), and the simplified version given by Eq. (1.81). We consider $|\epsilon| = 0.9$, and different values of the parameter $\Delta_\pm = \bar{r} \pm \bar{r}_{12}$. We also include results in absence of nonuniversal corrections to the interactions from Eq. (1.81), $\bar{\mathcal{E}}_D$. The values of $\Delta_\pm$ have been chosen to obtain lower energies per particle compared to conventional droplets. This behavior is in qualitatively agreement to Monte Carlo results for conventional droplets [24]. The repulsion-attraction balance that gives rise to 1d DNUC is metastable if the nonuniversal correction to the repulsion exceeds the nonuniversal correction of the attraction. Such a balance is broken providing $\Delta_- \gtrsim 4.5 \times 10^{-4}$ in Eq. (1.81). The DNUC becomes unstable and it is not possible to achieve a self-bound state. In Eq. (1.80) with $\Delta_- > 0$ there is a similar behavior, but the instability occurs faster due to the presence of the term with the factor Δ_+.

Using Eq. (1.79) we obtain the improved 1d GPE describing free droplets with nonuniversal corrections to the interactions as

$$\begin{aligned} i\hbar\frac{\partial\phi}{\partial t} &= \Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\delta g_-^{(0)}|\phi|^2 - \frac{1}{2}\delta g_+^{(2)}\frac{\partial^2}{\partial x^2}|\phi|^2 \\ &- \frac{1}{3\sqrt{2}\pi}\left(\frac{m}{\hbar^2}\right)^{1/2}\Big[[\delta g_-^{(0)}]^{3/2}F_+ + [\delta g_+^{(0)}]^{3/2}F_-\Big]|\phi|\Big]\phi, \end{aligned} \tag{1.82}$$

with $\delta g_\pm^{(0)} = |g^{(0)}| \pm |g_{12}^{(0)}| > 0$, $\delta g_\pm^{(2)} = g^{(2)} \pm g_{12}^{(2)}$, and

$$F_\pm = \frac{2 + f_\pm}{2f_\pm^2}, \qquad f_\pm = 1 + \frac{2m}{\hbar^2}[g^{(2)} \pm g_{12}^{(2)}]\phi^2. \tag{1.83}$$

The simplified version of this last expression taking into account the Petrov's approximation is given by

$$\begin{aligned} i\hbar\frac{\partial\phi}{\partial t} &= \Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\delta g_-^{(0)}|\phi|^2 - \frac{1}{2}\delta g_+^{(2)}\frac{\partial^2}{\partial x^2}|\phi|^2 \\ &- \frac{2}{3\pi}\left(\frac{m}{\hbar^2}\right)^{1/2}[g^{(0)}]^{3/2}F_-|\phi|\Big]\phi. \end{aligned} \tag{1.84}$$

From Eqs. (1.75) and (1.76) we can see that at level of mean-field approximation the nonuniversal contribution to the interactions provides a repulsive contribution. Increasing the density could be possible to find a critical value of $\delta g_\pm^{(2)}$ such that the mixture becomes unstable. This instability arises providing that the density of particles satisfies $|\phi|^2 = 1/[2(r \pm r_{12})]$, with $r > r_{12}$ choosing the negative sign. Therefore these two improved GPEs could be also useful to understanding the role of nonuniversal corrections to the interactions into properties of dark and bright solitons.

1.5.1 One-dimensional finite-temperature effects

In the continuum limit the $1d$ one-loop correction to the grand potential in expression (1.18) leads to [51]

$$\frac{\Omega_{\rm GF}^{(T)}}{L} = -\frac{1}{\pi}\sum_{\pm}\int_0^\infty dE_\pm(k_\pm)\frac{k_\pm}{e^{\beta E_\pm(k)}-1}, \tag{1.85}$$

with $k_\pm^2$ given by Eqs. (1.44) and (1.45). After introducing the variables $x_\pm = \beta E_\pm$, and expanding $k_\pm$ at low temperature $k_B T \ll |\mu|$ [44, 45], the $1d$ grand-canonical potential can be read as

$$\begin{aligned}\frac{\Omega_{\rm GF}^{(T)}}{L} &= -\frac{\pi}{6}\left(\frac{m}{\hbar^2}\right)^{1/2}\frac{(k_BT)^2}{\mu^{1/2}}\left[1-\frac{\pi^2}{20}\frac{(1+\delta_+\mu)}{\mu^2}(k_BT)^2\right] \\ &- \frac{\pi}{6}\left(\frac{m}{\hbar^2}\right)^{1/2}\frac{(k_BT)^2}{\lambda^{1/2}\mu^{1/2}}\left[1-\frac{\pi^2}{20}\frac{(1+\delta_-\mu)}{\lambda^2\mu^2}(k_BT)^2\right],\end{aligned} \tag{1.86}$$

and the respective thermal contribution to the energy per particle is

$$\begin{aligned}\frac{E^{(T)}}{N} &= \frac{\sqrt{2}\pi}{12}\left(\frac{m}{\hbar^2}\right)^{1/2}\frac{(k_BT)^2}{[g^{(0)}+g_{12}^{(0)}]^{1/2}n^{3/2}}(1+h_{NUC}^+) \\ &+ \frac{\sqrt{2}\pi}{12}\left(\frac{m}{\hbar^2}\right)^{1/2}\frac{(k_BT)^2}{[g^{(0)}-g_{12}^{(0)}]^{1/2}n^{3/2}}(1+h_{NUC}^-),\end{aligned} \tag{1.87}$$

with

$$h_{NUC}^\pm = -\frac{\pi^2}{5}\frac{(k_BT)^2}{[g^{(0)}\pm g_{12}^{(0)}]^2n^2}\left[1+\frac{6m}{\hbar^2}(g^{(2)}\pm g_{12}^{(2)})n\right]. \tag{1.88}$$

Clearly the $1d$ energy per particle in Eq. (1.87) is divergent providing $g^{(0)} = \pm g_{12}^{(0)}$. For attractive inter-species interactions lightly larger than repulsive intra-species interaction this energy per particle becomes complex, just like in $2d$ and $3d$ mixtures. In this sense we have a thermal-induced instability. However, even more remarkably instead both $1d$ DNUC and usual $1d$ droplets need to satisfy $g^{(0)} + g_{12}^{(0)} > 0$ and holds $g^{(0)} > \pm g_{12}^{(0)}$. Therefore both are stable at finite temperature. Currently, the region of greatest interest in the study of droplets is around $-g_{12} \sim$

g, so expression (1.87) is simplified dropping out to the second line. We also mention that the nonuniversal corrections to the interactions appear only up at order T^4 and, hence at very low temperatures these could be neglected.

1.6 Summary and outlook

In the framework of a quantum effective field theory we derive the equation of state at zero and low temperature of $3d$, $2d$ and $1d$ ultracold Bose-Bose mixtures of alkali-metal atoms considering nonuniversal corrections to the interactions. We perform one-loop Gaussian functional integration. The zero-point energy ultraviolet divergence is removed through dimensional regularization in $3d$ and in $1d$. In $2d$ we deal this issue by means of dimensional regularization in the modified minimal subtraction scheme. We stress and focus our analysis on the study of some regimes which the mixture manifests the existence and stable formation of a liquidlike phase with nonuniversal corrections to the interactions. In particular, when the nonuniversal contribution to the attraction exceeds that of repulsion in $3d$ DNUC, it results in an increasing in the equilibrium density regarding to the theoretical model to describe conventional droplets. The increase in the nonuniversal effect to the attraction causes the droplet to be unstable, and it disappears. The opposite happens when the nonuniversal correction to the attraction is exceeded by the repulsive counterpart. The equilibrium density and the respective minimum energy are lower than conventional droplet and there is not instability. If we consider the nonuniversal contributions as fitting parameters we found a good agreement from our model with some DMC results. In $2d$ DNUC we have found small deviations from the equilibrium density regarding usual droplets. A possible explanation for this could be associated with the coupling constants used. Due the perturbative nature of the self-bound liquidlike phase could be suitable consider coupling constants for $a \ll r$. In the $1d$ DNUC we obtain a qualitatively agreement with the trend of Monte Carlo results for conventional droplets. A clear extension of this work is verify the validity of our results by means of quantum Monte Carlo techniques [47, 48, 104]. We also propose some improved GPEs in $3d$, $2d$ and $1d$ including the enhanced nonuniversal contribution to the interactions. In these equations the parameter handling could be suitable for fitting with experimental or numerical evidence. Likewise, we consider that these equations could be useful in the study of the effects of the nonuniversal corrections to the interactions in paradigms that apply broadly to many-body quantum systems, as solitons and vortices. Given the experimental relevance of harmonic trapping potentials to achieve quasi-2d or quasi-1d regimes, it would be interesting not only to study harmonically trapped Bose-Bose mixtures including the nonuniversal corrections to the interactions, but also properties of DNUC at dimensional crossovers. We also consider that our theoretical predictions could stimulate experimental breakthroughs in the study in its own right of Gaussian fluctuations with nonuniversal corrections to the interactions in Bose-Bose mixtures. Sizable nonuniversal effects could be reached experimentally through Feshbach-resonance technique by increasing the density and decreasing the scattering length.

Finite-temperature effects deserve a further study on their own right. In principle in the droplet phase with or without nonuniversal corrections to the interactions both in 3d and in 2d, one could have the presence of a phase transition, even if the mixture is stable at zero temperature. For the 1d mixture could be interesting to see the thermal mechanisms driving the liquid-to-gas transition introduced in [65]. As our finite-temperature results are general for a symmetric Bose-Bose mixture could be interesting see how behaves the miscibility-separation condition regarding zero-temperature results [44, 45]. Our finite-temperature results could be contrasted with the recently implemented Monte Carlo methods at finite temperature [76, 77, 78]. In 3d we consider two different expansions of the phase shift, the conventional one, given in Eq. (1.24) and holding $a \gg r$ and a less known in Eq. (1.32) for $a \ll r$. From a scattering perspective it would be interesting to have expressions in the regime $a \ll r$ for both 2d and 1d, and also consider their effects on the liquidlike phase with nonuniversal corrections to the interactions.

Chapter 2

Droplets in Rabi-coupled nonuniversal Bose-Einstein condensates

Through an effective quantum field theory including zero temperature Gaussian fluctuations we derive analytical and explicit expressions for the equation of state of three-dimensional ultracold Rabi-coupled two-component bosonic gases with nonuniversal corrections to the interactions. At mean-field level the system presents two ground-states, one symmetric and one non-symmetric or unbalanced. For the symmetric ground state, in the regime where inter-species interactions are weakly attractive and subtly higher than repulsive intra-species, the instability by collapse is avoided by the contribution arising from Gaussian fluctuations, driving thus to formation of a liquidlike phase or droplet phase. This self-bound state is crucially affected by the dependence on the nonuniversal corrections to the interactions, which acts controlling the droplet stability. By tuning the ratio between the inter-species scattering length and the intra-species scattering lengths or the nonuniversal contribution to the interactions we address and establish conditions under which the formation and stability of self-bound Rabi-coupled droplets with nonuniversal corrections to the interactions is favorable. This chapter is based on Ref. [105].

2.1 Introduction

The coupling and handling among atomic hyperfine states by means of laser beams have become in a powerful tool leading to the possibility of inducing artificial transitions among such states [12, 13, 14]. An extensive experimental, theoretical and numerical research has been addressed to understand the properties of these synthetic non-Abelian gauge fields in neutral bosonic mixtures of ultracold gases [106, 107, 108, 109, 110, 111, 112, 113, 114]. It is remarkable to mention that most of theoretical developments have been carried out within the mean-field approximation by employing coupled Gross-Pitaevskii equations. As a result of these breakthroughs there is currently a wide field of research in spin-orbit- and Rabi-coupled ultracold bosonic atoms. A few years after arising of these artificial systems, and in the context of Gaussian fluctuations in Bose-Bose mixtures a new matter phase was proposed [23, 24]. This intriguing liquidlike state or droplet state lies in the highly nontrivial and subtle mechanical stabilization of paradigmatic mean-field collapse threshold in attractive condensed Bose-Bose mixtures through the repulsive Gaussian correction coming from zero-point motion of Bogoliubov excitations. Such a balance has revealed thus the crucial role played by fluctuations. This droplet phase has allowed the birth and fast development of a new field of research [50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 115]. Taking into account also the study of vortices, for example, in Ref. [100] it was shown that due to the effect of the logarithmic factor in two-dimensional droplets, the stable vortex droplets manifest a flat-top shape with embedded vorticity between 1 and 5. The spontaneous symmetry breaking in one-dimensional droplets loaded in a symmetric double-core cigar-shaped potential is also considered in Ref. [116]. The results show droplets feature flat-top profiles for large values of total norm, and bell (sech)-shaped density profiles for smaller values of total norm.

It is noteworthy that though the fluctuations are usually small, these can be experimentally tuning by means of Feshbach resonances. Thus experimental evidence has been obtained regarding outstanding influence of this small corrections. Experimental droplets has been obtained in ^{39}K-^{39}K mixtures [25, 26, 27, 28] and ^{41}K-^{87}Rb mixtures [29]. Also has been studied the dynamical formation of self-bound droplets in attractive mixture of ^{39}K atoms [30]. More recently the observation of a Lee-Huang-Yang (LHY) fluid in a ^{39}K spin mixture confined in a spherical trap potential has been achieved [31]. Droplets also have been obtained in a mixture of ^{23}Na and ^{87}Rb with tunable attractive inter-species interactions [32]. Shortly after the theoretical proposal of Bose-Bose droplets, this idea was extended both at experimental and theoretical level to the context of one-component Bose gases with magnetic atoms, [33, 34, 35, 36, 37, 38, 39, 70, 71, 72, 73]. More recently a numerical study of stable three-dimensional anisotropic dipolar droplets with embedded vorticity and composite states with the vortex-antivortex-vortex structure is performed in Ref. [117]. However, fitting experimental results with theoretical predictions some discrepancies have been found for both Bose-Bose droplets and droplets in bosonic dipolar gases. In fact, in three-dimensional Bose-Bose gases it was observed that a minimum number of atoms is required to achieve a stable droplet formation [25], and this value is less than predicted in Ref. [23]. Some differences have also been found between the theoretical model and Monte Carlo results in Bose-Bose droplets [46, 47, 48]. In an attempt to achieve a better description of this phase a phenomenological beyond Lee-Huang-Yang (LHY) framework has been developed in [74], for Bose-Bose droplets in three and one dimension. Therefore, given the discrepancies with both experimental and numerical results, a better description of this phenomenon remains as an open issue. From a theoretical framework, it is worth noting that both Bose-Bose droplets and bosonic dipolar droplets remain weakly interacting, allowing thus for a theoretical perturbative treatment. In such a scenario for two-component bosonic droplets a key ingredient is to consider the weakly interactions approximated by a local contact interaction. In this sense, only the s-wave scattering length characterizes the two-body interatomic interactions, and we have an universal regime [49]. On the other hand, if the physical quantities depend on properties other than the s-wave scattering length we have a nonuniversal regime. In addition and due to the sensitive nature of the fluctuations themselves the effect of some other parameter on these remains as an open issue.

Therefore taking into account the above mentioned, a connection between artificial spinor condensates and droplets is an interesting not widely explored research field. In this sense a first attempt to connect these two fields of research has been carried out in Refs. [55, 115]. In these works the coherent coupling between two atomic internal states provided by Rabi coupling and droplets in two-component Bose gases of interacting alkali-metal atoms was investigated. More recently, experimental measures of fluctuations with vanishing mean-field energy in an asymmetric Rabi-coupled Bose-Einstein condensate with atoms of ^{39}K in a waveguide have been carried out in Ref. [118]. So, for a better understanding of fluctuations behavior on Rabi-coupled Bose-Bose mixtures and motivated by the enhanced role of these, we consider an extra ingredient. We propose a step beyond by researching the effect of the nonuniversal corrections to the interactions [75, 83] on Rabi-coupled bosonic droplets. Recently, Bose-Bose gases with such a kind of corrections to the interactions in three, two, and one dimension both at zero and finite temperature have been considered in Ref. [50]. It has been shown as the nontrivial dependence on the nonuniversal corrections to the interactions crucially affects the self-bound droplets stability. Hence we address theoretically on the zero temperature nonuniversal equation of state for three-dimensional Rabi-coupled bosonic gases and we focus on the formation and stability of self-bound

Rabi-coupled Bose-Bose droplets with nonuniversal corrections to the interactions.

The rest of the chapter is organized as follows. In Section 2.2 we introduce an effective-field theory in the path-integral formalism to describe interacting Rabi-coupled bosons with nonuniversal corrections to the interactions. We derive the mean-field grand-canonical potential, and we establish some conditions under which it is possible to obtain analytical expressions for the ground state. In fact, we present two different kind of ground states one symmetric and one non-symmetric or unbalanced. We calculate the leading contribution to the equation of state for the symmetric ground-state at level of the Gaussian fluctuations at zero temperature in section 2.3. As a starting point in the first part of this section we analyze some aspects of the Gaussian fluctuations in absence of the nonuniversal corrections to the interactions. We consider the three-, two- and one-dimensional cases, with the particularities of each dimension. These particularities are mainly associated with the best way to address the issue of ultraviolet divergences. We also present some comments related to the droplet phase in each dimension. In the second part of section 2.3 we focus on the three dimensional Gaussian fluctuations of the nonuniversal Rabi coupled bosons. In order to obtain closed analytical expressions useful simplifications take place when, in the spectrum, we make use of the physically reasonable approximation of weak Rabi frequency, $\omega_R \ll \mu/\hbar$ [119]. We perform dimensional regularization to solve the divergent zero-point integrals due to both gapless and gapped elementary excitations. Here we analyze the conditions for the existence of a stable formation of droplets with attractive inter-species scattering length and repulsive intra-species scattering length. In such a case, we obtain an analytical expression for the energy density of nonuniversal Rabi-coupled bosonic droplets with a nontrivial dependence of scattering lengths, nonuniversal effects of the interactions, and the Rabi coupling. We also include some phase diagrams relating some of the parameters above mentioned. In section 2.4 we draw a final discussion and we present some future perspectives of our results.

2.2 An effective-field theory for Nonuniversal Rabi-coupled bosons

In this section we introduce some elements of interest in the path-integral formalism, see appendix A. This functional formalism is equivalent to the creation and annihilation operators procedure [88, 90]. Fluctuations in three-dimensional ($3d$) one-component bosonic gases with hard-sphere interactions were originally considered in [120, 121]. In such a work the LHY-corrections were obtained using the formalism of creation and annihilation operators. In the context of fluctuations in two-component bosonic gases, the same operators procedure it was considered in Refs. [23, 24, 122]. On the other hand, same results were obtained into the path-integral formalism in Ref. [51]. So, we consider $3d$ equal-mass two-component Rabi-coupled ultracold bosonic gases with nonuniversal corrections to the interactions and chemical potential μ, in the path-integral formalism. The action in a $3d$ box of volume V can be read as [50, 115]

$$
\begin{aligned}
S[\Psi,\Psi^*] &= \sum\!\!\!\!\!\!\int \Big[\psi_\alpha^*(\mathbf{r},\tau)\big(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 - \mu\big)\psi_\alpha(\mathbf{r},\tau) \\
&+ \frac{1}{2}\sum_\sigma g_{\alpha\sigma}^{(0)}|\psi_\alpha(\mathbf{r},\tau)|^2|\psi_\sigma(\mathbf{r},\tau)|^2 \\
&- \frac{1}{2}\sum_\sigma g_{\alpha\sigma}^{(2)}|\psi_\alpha(\mathbf{r},\tau)|^2\nabla^2|\psi_\sigma(\mathbf{r},\tau)|^2 \\
&- \hbar\omega_R(\psi_1^*\psi_2 + \psi_2^*\psi_1)\Big],
\end{aligned} \tag{2.1}
$$

where we have used the shorthand notation $\sum\!\!\!\!\!\int \equiv \int_0^{\hbar\beta} d\tau \int_V d^3r \sum_\alpha$, $\beta = 1/k_BT$, k_B is the Boltzmann constant, and the hyperfine states are labeled as $\alpha,\sigma = 1,2$. Each component is described by a complex bosonic field ψ_α, and these fields are considered at position $\mathbf{r}$ and imaginary time τ. The superscripts $(0,2)$ are related to the zero-range approximation to the interactions and the nonuniversal improvements to the interactions, respectively. Dealing with ultracold and dilute bosons, the most common scheme to taking into account the interactions is to consider an approximated zero-range potential [44, 45]. Hence, the strength of the interactions is expressed through the intra- and interspecies coupling constants $g_{\alpha\alpha}^{(0)} = 4\pi\hbar^2 a_{\alpha\alpha}/m$ and $g_{\alpha\sigma}^{(0)} = 4\pi\hbar^2 a_{\alpha\sigma}/m$, respectively. These in turn are related to the s-wave scattering lengths $a_{\alpha\alpha}$ and $a_{\alpha\sigma}$, respectively, such that $a_{\alpha\alpha}, a_{\alpha\sigma} > 0$ represent repulsion, and $a_{\alpha\alpha}, a_{\alpha\sigma} < 0$ attraction. In order to research the role played by the effects beyond the zero-range approximation to the interactions, we include the nonuniversal corrections to the two-body interatomic interaction potential in the third line of Eq. (2.1). Thus we have the coupling constants for intra-species and inter-species with nonuniversal corrections to the interactions $g_{\alpha\alpha}^{(2)}$ and $g_{\alpha\sigma}^{(2)}$, respectively. It is remarkable mentioning that from scattering theory there are two different coupling constants considering the s-wave effective range of interaction

r, such that [93, 94, 95]

$$g^{(2)}_{\alpha\alpha} = \frac{2\pi\hbar^2}{m} a^2_{\alpha\alpha} r_{\alpha\alpha} \qquad\qquad a_{\alpha\alpha} \gg r_{\alpha\alpha}, \tag{2.2}$$

$$g^{(2)}_{\alpha\sigma} = \frac{2\pi\hbar^2}{m} a^2_{\alpha\sigma} r_{\alpha\sigma} \qquad\qquad a_{\alpha\sigma} \gg r_{\alpha\sigma}, \tag{2.3}$$

and, [96]

$$g^{(2)}_{\alpha\alpha} = -\frac{2\pi\hbar^2}{3m} r^3_{\alpha\alpha} \qquad\qquad a_{\alpha\alpha} \ll r_{\alpha\alpha}, \tag{2.4}$$

$$g^{(2)}_{\alpha\sigma} = -\frac{2\pi\hbar^2}{3m} r^3_{\alpha\sigma} \qquad\qquad a_{\alpha\sigma} \ll r_{\alpha\sigma}. \tag{2.5}$$

These last with a good numerical description of low-energy scattering. In absence of the Rabi coupling, a better description of the droplet phase is achieved by considering the couplings (2.4), and (2.5), see Ref. [50]. From now on we will take into account these couplings. Transitions between the two states are induced by an external coherent Rabi coupling of frequency $\omega_R > 0$. Due to the Rabi mixing between states, only the total number of particles is conserved [123]. Thus it is assumed that the two components are in a state with the same chemical potential μ [123, 124, 125].

In order to obtain the ground state of the system, we calculate the grand potential $\Omega = -\beta^{-1} \ln \mathcal{Z}$. In the path-integral formalism the grand canonical partition function $\mathcal{Z}$ at temperature T is written as

$$\mathcal{Z} = \int \mathcal{D}[\Psi, \Psi^*] \exp(-S[\Psi, \Psi^*]/\hbar). \tag{2.6}$$

At zero temperature we assume the bosons condensate into the zero-momentum states. In other words, we consider the superfluid phase, where a $U(1)$ gauge symmetry of each component is spontaneously broken. So in order to performing a perturbative expansion we set $\psi_\alpha(\mathbf{r}, \tau) = \phi_\alpha + \eta_\alpha(\mathbf{r}, \tau)$ [115]. Where $\phi_\alpha \equiv \langle \psi_\alpha(\mathbf{r}, \tau) \rangle$ [88], corresponds to the condensate wave-function. The fluctuations around ψ_α are given by $\eta_\alpha(\mathbf{r}, \tau)$ and these are orthogonal to the condensate of the same species [88, 89]. Here we have $n_\alpha = |\phi_\alpha|^2 = N_\alpha / L^d$, as the density of particles in the mean-field approximation or macroscopic density of the Bose-

Einstein condensate. After introducing $\psi_\alpha(\mathbf{r},\tau) = \phi_\alpha + \eta_\alpha(\mathbf{r},\tau)$ into the action (2.1) we expand the action up to the second order (Gaussian) in $\eta_\alpha(\mathbf{r},\tau)$ and $\eta^*_\alpha(\mathbf{r},\tau)$, and we arrive at the split grand potential $\Omega = \Omega_0 + \Omega_{\mathrm{GF}}$. Where Ω_0 is the mean-field contribution, while Ω_{f} takes into account the Gaussian zero-temperature fluctuations. Since ϕ_α describes the condensate, the linear terms in the fluctuations vanish such that ϕ_α really minimizes the action [88]. Thus the explicit form of the mean-field grand-potential could be obtained by minimizing the mean-field grand potential Ω_0 with respect to ϕ (saddle-point approximation), as will be seen later.

2.2.1 Mean-field ground states

At first instance we carry out the analysis of the mean-field contribution, where $\psi_\alpha = \phi_\alpha$, from which we get the following grand-potential

$$\frac{\Omega_0}{V} = \sum_{\alpha=1,2} \Big(-\mu\phi_\alpha^2 + \frac{1}{2}\sum_{\sigma=1,2} g^{(0)}_{\alpha\sigma}\phi_\alpha^2\phi_\sigma^2 \Big) - 2\hbar\omega_R\phi_1\phi_2, \tag{2.7}$$

which is not dependent on the nonuniversal effects of the interactions, given the derivative of the nonuniversal contribution in Eq. (2.1). In the saddle-point approximation i.e., minimizing Ω_0 with respect to ϕ_α, we obtain

$$\mu\phi_\alpha = \big(g^{(0)}_{\alpha\alpha}\phi_\alpha^2 + g^{(0)}_{\alpha\sigma}\phi_\sigma^2\big)\phi_\alpha - \hbar\omega_R\phi_\sigma, \tag{2.8}$$

with $\alpha,\sigma = 1,2$ and $\alpha \neq \sigma$. In addition useful simplifications take place when the intra-species are equal, such that, $g^{(0)}_{11} = g^{(0)}_{22} = g^{(0)} = 4\pi\hbar^2 a/m$. Therefore solving Eq. (2.8) we get

$$\big[\big(g^{(0)} - g^{(0)}_{12}\big)\phi_1\phi_2 + \hbar\omega_R\big]\big(\phi_1^2 - \phi_2^2\big) = 0. \tag{2.9}$$

Since $|\phi_1|^2 = n_1$, and $|\phi_2|^2 = n_2$ are the densities of each internal state, the total density is given as $n = n_1 + n_2$. Thus two solutions of Eq. (2.9) are obtained. One is a symmetric phase where the two internal states are equally populated $n_1 = n_2$. The other solution is a non-symmetric or unbalanced configuration which exists only in presence of the Rabi coupling and it arises when the intra- and inter-spin interactions of the two species are not equal, leading thus to a non-zero spin density polarization $n_1 - n_2$. Now briefly we describe some general aspects related to these ground-states [115].

Symmetric ground-state

In the symmetric phase we consider $n_1 = n_2 = n/2$, and from Eq. (2.8) we get

$$n = \frac{2\mu_R}{g^{(0)} + g_{12}^{(0)}}, \tag{2.10}$$

where $\mu_R = \mu + \hbar\omega_R$, and the corresponding mean-field grand-potential can be read as

$$\frac{\Omega_0}{V} = -\frac{\mu_R^2}{g^{(0)} + g_{12}^{(0)}}, \tag{2.11}$$

with the respective mean-field energy density $\mathcal{E}_0$ given by

$$\mathcal{E}_0 = \frac{1}{4}\big(g^{(0)} + g_{12}^{(0)}\big)n^2 - \hbar\omega_R n, \tag{2.12}$$

where we can see that the minimum value of the energy density to obtain the stable symmetric ground-state $\mathcal{E}_{0,\text{min}} = -\hbar^2\omega_R^2/(g^{(0)} + g_{12}^{(0)})$ is handled by the Rabi frequency. In this symmetric ground-state the Hessian matrix indicates that the grand-potential stability at mean-field level in Eq. (2.7) is achieved satisfying the condition

$$\big(g^{(0)} + g_{12}^{(0)}\big)\big[\big(g^{(0)} - g_{12}^{(0)}\big)\mu + 2\hbar\omega_R g^{(0)}\big] > 0. \tag{2.13}$$

In Fig. 2.1 we show the existence condition for the symmetric ground-state given by (2.13). In this phase, Eq. (2.10) establishes $\mu/\hbar\omega_R > -1$ in order to have a physical density $n > 0$. Without Rabi coupling it is know that for a complete set of repulsive interactions, where $g^{(0)} > 0$ and $g_{12}^{(0)} > 0$, in order to ensure a stable miscibility phase (overlapping of two components), and avoiding the phase separation, it is necessary providing $0 < g_{12}^{(0)}/g^{(0)} < 1$ [44, 45]. In the phase separation the repulsion between atoms belonging to the same species is stronger that repulsion between species and as consequence there is not mixing between two species. However, the inclusion of Rabi coupling gives rise to an effective attraction between the species which can drive the immiscible configuration into a miscible state, and the stable ground-state remains. On the other hand, at mean-field level a condensed Bose-Bose mixture in absence of Rabi coupling collapses when the interspecies attraction $g_{12}^{(0)} < 0$ becomes stronger than intraspecies repulsion, $g^{(0)} > 0$, providing $[g_{12}^{(0)}]^2 > [g^{(0)}]^2$ with $-1 < g_{12}^{(0)}/g^{(0)} < 0$. In such

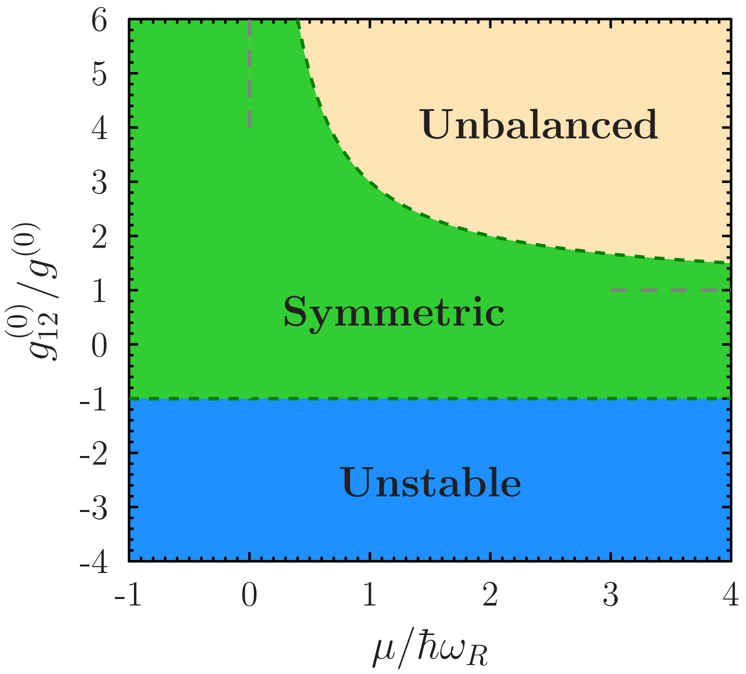

Figure 2.1: Ground states mean-field phase diagram of interacting Rabi-coupled bosons [115]. Symmetric region is given by condition (2.13), and the unbalanced or non-symmetric region is obtained from condition (2.17). The ratio value $g_{12}^{(0)}/g^{(0)} = 1$ represents the asymptotic behavior for large values of $\mu/\hbar\omega_R$ (horizontal dashed gray line), and $\mu/\hbar\omega_R = 0$ represents the asymptotic behavior for large $g_{12}^{(0)}/g^{(0)}$ ratio (vertical dashed gray line).

a case this attractive mechanism is leading and there is not an effect of the Rabi contribution. The mixture remains unstable for $g_{12}^{(0)}/g^{(0)} < -1$, blue region in Fig. 2.1.

Unbalanced or Non-symmetric ground-state

In the non-symmetric phase using the second solution from Eq. (2.9) into Eq. (2.8), the density of each state can be read as

$$n_{1,2} = \frac{\mu}{2g^{(0)}}\left[1 \pm \sqrt{1 - \left[\frac{2\hbar\omega_R g^{(0)}}{\left(g^{(0)} - g_{12}^{(0)}\right)\mu}\right]^2}\right] \tag{2.14}$$

such that $n = \mu/g^{(0)}$. The Rabi coupling presence destabilizes the symmetric ground-state allowing thus the arising of this unbalanced phase. So the mean-field grand potential can be read as

$$\frac{\Omega_0}{V} = -\frac{1}{2}\frac{\mu^2}{g^{(0)}} + \frac{(\hbar\omega_R)^2}{g^{(0)} - g_{12}^{(0)}}, \tag{2.15}$$

with the respective mean-field energy density given by

$$\mathcal{E}_0 = \frac{1}{2}g^{(0)}n^2 + \frac{(\hbar\omega_R)^2}{g^{(0)} - g_{12}^{(0)}}, \tag{2.16}$$

where the Rabi coupling contribution acts as an shift of the mean-field energy density of a single Bose-Einstein condensate. The coupling constants also impose the condition $g^{(0)} \neq g_{12}^{(0)}$ for the existence of the unbalanced ground-state. From Eq. (2.7) the stability of the non-symmetric ground-state is obtained providing

$$\left(g^{(0)} - g_{12}^{(0)}\right)\left[4g^{(0)} - \frac{\left(g^{(0)} - g_{12}^{(0)}\right)^2\mu^2}{g^{(0)}(\hbar\omega_R)^2}\right] > 0, \tag{2.17}$$

as it is shown in the Fig. 2.1.

2.3 Gaussian fluctuations of the symmetric ground-state

2.3.1 Gaussian fluctuations in absence of the nonuniversal corrections to the interactions

Hereafter, we focus on the symmetric configuration. For simplicity we first initially consider the case in the absence of nonuniversal corrections to the interactions for $d = 3$ [115], and the lower dimensional scenario $d = 2, 1$ [55]. Later, extending this analysis, we included such a nonuniversal corrections and we analyze the case $d = 3$. The grand potential of the Gaussian fluctuations Ω_{GF} is provided by [82]

$$\Omega_{\text{GF}} = \frac{1}{2\beta}\sum_{k>0}\sum_{n=-\infty}^{+\infty} \ln\det[\mathbb{G}^{-1}(k,\omega_n)], \tag{2.18}$$

with the bosonic Matsubara's frequencies $\omega_n = 2\pi n/(\hbar\beta)$, and the 4×4 inverse fluctuation propagator $\mathbb{G}^{-1}$ given as

$$\mathbb{G}^{-1}(k,\omega_n) = \tag{2.19}$$

$$\begin{pmatrix} -i\hbar\omega_n + f_1(k) & \frac{g}{g+g_{12}}\mu_R & \frac{g_{12}}{g+g_{12}}\mu_R - \hbar\omega_R & \frac{g_{12}}{g+g_{12}}\mu_R \\ \frac{g}{g+g_{12}}\mu_R & i\hbar\omega_n + f_1(k) & \frac{g_{12}}{g+g_{12}}\mu_R & \frac{g_{12}}{g+g_{12}}\mu_R - \hbar\omega_R \\ \frac{g_{12}}{g+g_{12}}\mu_R - \hbar\omega_R & \frac{g_{12}}{g+g_{12}}\mu_R & -i\hbar\omega_n + f_1(k) & \frac{g}{g+g_{12}}\mu_R \\ \frac{g_{12}}{g+g_{12}}\mu_R & \frac{g_{12}}{g+g_{12}}\mu_R - \hbar\omega_R & \frac{g}{g+g_{12}}\mu_R & i\hbar\omega_n + f_1(k) \end{pmatrix}, \tag{2.20}$$

where

$$f_1(k) = \frac{\hbar^2 k^2}{2m} + \Big(\frac{2g + g_{12}}{g + g_{12}}\Big)\mu_R - \mu. \tag{2.21}$$

The determinant of the inverse propagator is

$$\begin{aligned} \det\mathbb{G}^{-1} &= \Big[\Big(\frac{\hbar^2 k^2}{2m}\Big)^2 + \frac{\hbar^2 k^2}{m}\mu_R\Big] \\ &\times \Big\{\Big[\frac{\hbar^2 k^2}{2m} + \Big(\frac{g - g_{12}}{g + g_{12}}\Big)\mu_R + 2\hbar\omega_R\Big]^2 - \Big(\frac{g - g_{12}}{g + g_{12}}\Big)^2 \mu_R^2\Big\}. \end{aligned} \tag{2.22}$$

So we obtain the Gaussian grand-canonical potential

$$\Omega_{\mathrm{GF}} = \frac{1}{2\beta} \sum_{\substack{k>0 \\ n=-\infty}}^{+\infty} \ln\big[(\hbar^2\omega_n^2 + E_+^2)(\hbar^2\omega_n^2 + E_-^2)\big], \tag{2.23}$$

with the respective Bogoliubov spectra given as

$$E_+ = \sqrt{\frac{\hbar^2 k^2}{2m}\Big(\frac{\hbar^2 k^2}{2m} + 2\mu_R\Big)}, \tag{2.24}$$

and

$$E_- = \sqrt{\frac{\hbar^2 k^2}{2m}\Big(\frac{\hbar^2 k^2}{2m} + 2\bar{A}\Big) + \bar{B}}, \tag{2.25}$$

where $\bar{A} = \Delta\mu_R + 2\hbar\omega_R$, $\bar{B} = 4(\Delta\mu_R + \hbar\omega_R)\hbar\omega_R$, and $\Delta = (g - g_{12})/(g + g_{12})$.

We neglect the finite-temperature contribution in the sum of Eq. (2.23) . So in the continuum limit the contribution at zero temperature in the sum of Eq. (2.23) is

$$\begin{aligned}\frac{\Omega_{\rm GF}}{L^d} &= \frac{1}{2(2\pi)^d}\frac{2\pi^{d/2}}{\Gamma(d/2)}\int_0^\infty dk\,k^{d-1}[E_+(k,\mu,\omega_R)+E_-(k,\mu,\omega_R)] \\ &= \frac{\Omega^+_{\rm GF}}{L^d}+\frac{\Omega^-_{\rm GF}}{L^d}. \end{aligned} \tag{2.26}$$

For $d=3$ and, $d=1$ we consider the small Rabi-coupling limit [115, 119]. In this limit we obtain closed expressions for these dimensions. However for $d=2$ it is possible to obtain a general form for any values of the Rabi coupling, as we will see later. So we first deal with $d=3,1$. It is worth mentioning that the ultraviolet divergence in the integral over E_+ can be treated directly by means of dimensional regularization whether for $d=3$, $d=2$ or $d=1$, see appendix D. On the other hand, for E_- we have that to linear order in the Rabi-coupling the integral over the E_- branch of the Bogoliubov spectra becomes

$$\begin{aligned}\frac{\Omega^-_{\rm GF}}{L^d} &= \frac{1}{2}\frac{S_d}{(2\pi)^d}\int dk\,k^{d-1}\Big\{\sqrt{\frac{\hbar^2k^2}{2m}\Big(\frac{\hbar^2k^2}{2m}+2\Delta\mu\Big)} \\ &+ \frac{\hbar\omega_R}{\sqrt{\frac{\hbar^2k^2}{2m}\Big(\frac{\hbar^2k^2}{2m}+2\Delta\mu\Big)}}\Big[(2+\Delta)\frac{\hbar^2k^2}{2m}+2\Delta\mu\Big]\Big\}+\mathcal{O}\Big(\Big(\frac{\hbar\omega_R}{\mu}\Big)^2\Big), \\ &\equiv I_1+I_2. \end{aligned} \tag{2.27}$$

By means of dimensional regularization we have

$$I_1=\frac{S_d(2\Delta\mu)^{(2+d)/2}}{4(2\pi)^d}\Big(\frac{2m}{\hbar^2}\Big)^{d/2}\frac{\Gamma\big(\frac{1+d}{2}\big)\Gamma\big(-\frac{2+d}{2}\big)}{\Gamma\big(-\frac{1}{2}\big)}, \tag{2.28}$$

and,

$$I_2=\frac{1}{4}S_d\hbar\omega_R\Big(\frac{m\Delta\mu}{\pi^2\hbar^2}\Big)^{d/2}\Big[(2+\Delta)\mathrm{B}\Big(\frac{1+d}{2},-\frac{d}{2}\Big)+\mathrm{B}\Big(\frac{d-1}{2},\frac{2-d}{2}\Big)\Big]. \tag{2.29}$$

For **d=3** we obtain

$$\frac{\Omega^-_{\rm GF}}{L^3}=\frac{8}{15\pi^2}\Big(\frac{m}{\hbar^2}\Big)^{3/2}(\Delta\mu)^{5/2}+\frac{2\hbar\omega_R}{3\pi^2}(1+2\Delta)\Big(\frac{m\Delta\mu}{\hbar^2}\Big)^{3/2}. \tag{2.30}$$

The integral over E_+ is

$$\frac{\Omega^{+}_{\rm GF}}{L^3} = \frac{8}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\mu_R^{5/2}. \tag{2.31}$$

For **d=1** the first contribution in Eq. (2.29) gives $-(2+\Delta)(m\mu\Delta)^{1/2}\omega_R/\pi$. However, it is necessary to be more careful with the second term in Eq. (2.29), (we named it as I_3). It is still divergent, so we use the $\overline{\rm MS}$-scheme. Thus through $d = 1-2\bar{\epsilon}$, we get

$$\begin{aligned} I_3 &= \frac{\omega_R}{2\pi}(m\mu\Delta)^{1/2}\left(\frac{\pi\hbar^2}{m\mu\Delta}\right)^{\bar{\epsilon}}\left(\frac{e^{\gamma}\kappa^2}{4\pi}\right)^{\bar{\epsilon}}\frac{\Gamma(-\bar{\epsilon})\Gamma(\frac{1}{2}+\bar{\epsilon})}{\Gamma(\frac{1}{2}-\bar{\epsilon})} \\ &= \frac{\omega_R}{2\pi}(m\mu\Delta)^{1/2}\left[-\frac{1}{\bar{\epsilon}}+\ln\left(\frac{64m\mu\Delta}{\hbar^2\kappa^2}\right)\right]+\mathcal{O}(\bar{\epsilon}). \end{aligned} \tag{2.32}$$

To obtain this result we use the same method that was applied to deal with Eq. (D.15). By taking into account the appropriate counterterms subtraction to remove the simple pole of the Gamma function encoded in $\bar{\epsilon}$, and applying the limit $\bar{\epsilon}\to 0$, we obtain

$$\frac{\Omega^{-}_{\rm GF}}{L} = -\frac{2}{3\pi}\left(\frac{m}{\hbar^2}\right)^{\frac{1}{2}}(\Delta\mu)^{\frac{3}{2}} - \frac{\omega_R}{\pi}(m\Delta\mu)^{1/2}\left[\Delta+\frac{1}{2}\ln\left(\frac{\hbar^2\kappa^2e^4}{64m\Delta\mu}\right)\right]. \tag{2.33}$$

The integral over E_+ is

$$\frac{\Omega^{+}_{\rm GF}}{L} = -\frac{2}{3\pi}\left(\frac{m}{\hbar^2}\right)^{1/2}\mu_R^{3/2}. \tag{2.34}$$

For **d=2** the integral over E_-, for any value of the Rabi frequency, is considered using convergence-factor regularization (CFR) [82, 115]. Now, defining $x^2 \equiv \hbar^2k^2/(2m)$, we have

$$\begin{aligned} \frac{\Omega^{-}_{\rm GF}}{L^2} &= \frac{m}{2\pi\hbar^2}\int_0^{\infty} dx\, x\left[\sqrt{x^4+2\bar{A}x^2+\bar{B}}-x^2-\bar{A}-\frac{1}{2x^2}(\bar{B}-\bar{A}^2)\right] \\ &= \frac{m}{2\pi\hbar^2}\left\{\frac{1}{4}\left[(\bar{B}-\bar{A}^2)\ln\left(\sqrt{x^4+2\bar{A}x^2+\bar{B}}+x^2+\bar{A}\right)\right.\right. \\ &+ \left.(\bar{A}+x^2)\sqrt{x^4+2\bar{A}x^2+\bar{B}}\right] \\ &- \left.\frac{1}{4}x^4-\frac{1}{2}\bar{A}x^2-\frac{1}{2}(\bar{B}-\bar{A}^2)\ln x\right\}\Bigg|_0^{\infty}. \end{aligned} \tag{2.35}$$

The logarithmic term in the second line can be written in a more convenient way as

$$\ln\Big[\frac{1}{2}\Big(\sqrt{x^2+2\bar{A}+\frac{\bar{B}}{x^2}}+x\Big)^2-\frac{\bar{B}}{2x^2}\Big], \tag{2.36}$$

and defining $\bar{\delta}\equiv(1-\sqrt{\bar{B}}/\bar{A})/(1+\sqrt{\bar{B}}/\bar{A})$, as a result we obtain the two-dimensional homogeneous grand-canonical potential for the branch E_- for any positive value of the Rabi frequency

$$\begin{aligned}\frac{\Omega^-_{\text{GF}}}{L^2} &= \frac{\bar{A}^2 m}{4\pi\hbar^2}\Big[\frac{1}{2}\Big(\frac{\bar{B}}{\bar{A}^2}-1\Big)\ln\Big(\frac{\hbar^2\kappa^2}{\bar{A}m}\Big)+\frac{1}{4}\Big(1+\frac{\bar{B}}{\bar{A}^2}-\frac{2\sqrt{\bar{B}}}{\bar{A}}\Big)\Big]\\ &= -\frac{\bar{A}^2 m}{8\pi\hbar^2}\Big(1-\frac{\bar{B}}{\bar{A}^2}\Big)\ln\frac{\hbar^2\kappa^2}{\bar{A}me^{\bar{\delta}/2}}\\ &= -\frac{m\Delta^2\mu_R^2}{8\pi\hbar^2}\ln\Big[\frac{\hbar^2\kappa^2 e^{-\bar{\delta}/2}}{m(\Delta\mu_R+2\hbar\omega_R)}\Big],\end{aligned} \tag{2.37}$$

By means of dimensional regularization we also have

$$\frac{\Omega^+_{\text{GF}}}{L^2} = -\frac{m}{8\pi\hbar^2}\mu_R^2\ln\Big(\frac{\hbar^2\kappa^2}{\sqrt{e}m\mu_R}\Big). \tag{2.38}$$

The independence of Ω/L^2 on the scale parameter κ is achieved since it is satisfied with Eq. (D.27). The integrals over E_+ and E_- for $d=3$ and $d=1$, in the limit of small Rabi frequency, or the integral over E_+ for $d=2$ can be also obtained by means of CFR, as we will see below. Taking into account that the integral that requires the most attention is given in the second line of the Eq. (2.27) we will focus on it. In other words we solve I_2. However, the integral over E_+ (for $d=3,2,1$) and the integral I_1 (for $d=3,1$) are expected.

So for **d=3** with $x^2=\hbar^2k^2/(2m)$, and using CFR we get

$$\begin{aligned} I_2 &= \frac{\hbar\omega_R}{(2\pi)^2}\Big(\frac{2m}{\hbar^2}\Big)^{3/2}\int_0^\infty dx\,\Big\{x\frac{[(2+\Delta)x^2+2\Delta\mu]}{\sqrt{x^2+2\Delta\mu}}\\ &- (2+\Delta)(x^2-\Delta\mu)-2\Delta\mu\Big(1-\frac{\Delta\mu}{x^2}\Big)\Big\}\\ &= \frac{\hbar\omega_R}{4\pi^2}\Big(\frac{2m}{\hbar^2}\Big)^{3/2}\Big\{(2+\Delta)\Big[\frac{1}{3}(2\Delta\mu)^{3/2}\Big[\frac{(x^2+2\Delta\mu)^{3/2}}{(2\Delta\mu)^{3/2}}-\frac{3(x^2+2\Delta\mu)^{1/2}}{(2\Delta\mu)^{1/2}}\Big]\\ &- \frac{1}{3}x^3+\Delta\mu x\Big]+2\Delta\mu\Big(\sqrt{x^2+2\Delta\mu}-x\Big)\Big\}\Big|_0^\infty.\\ &= \frac{2}{3\pi^2}(1+2\Delta)\Big(\frac{m\Delta\mu}{\hbar^2}\Big)^{3/2}\hbar\omega_R. \end{aligned} \tag{2.39}$$

The same result as in the last term of Eq. (2.30) where it was applied dimensional regularization.

So for **d=1** with $x^2 = \hbar^2 k^2/(2m)$, and using CFR we get

$$\begin{aligned} I_2 &= \frac{\omega_R}{2\pi}\sqrt{2m}\int_0^{\infty} dx\Big[(2+\Delta)\Big(\frac{x}{\sqrt{x^2+2\Delta\mu}}-1\Big)+\frac{2\Delta\mu}{x\sqrt{x^2+2\Delta\mu}}\Big] \\ &= \frac{\omega_R}{2\pi}\sqrt{2m}\Big[(2+\Delta)\Big[\sqrt{x^2+2\Delta\mu}-x\Big] \\ &- \sqrt{2\Delta\mu}\ln\Big(\frac{\sqrt{x^2+2\Delta\mu}+\sqrt{2\Delta\mu}}{x}\Big)\Big]\Big|_0^{\infty} \\ &= -\frac{\omega_R}{\pi}(m\mu\Delta)^{1/2}\Big[\Delta+\frac{1}{2}\ln\Big(\frac{\hbar^2\kappa_{CFR}^2 e^4}{16m\Delta\mu}\Big)\Big]. \end{aligned} \tag{2.40}$$

For this integral we find equivalence between dimensional regularization and the CFR as long as $\kappa_{\mathrm{MS}}^2 = 4\kappa_{\mathrm{CFR}}^2$.

The three-dimensional droplet

Now, by taking $E_B = \hbar^2/ma^2$ as energy unit, with the Rabi frequency $\widetilde{\omega}_R E_B = \hbar\omega_R$, the density $\widetilde{n} = na^3$, the energy density $\mathcal{E} = E/V$, and the ratio $\epsilon = g_{12}/g$. This leads to the total scaled energy density per particle $\widetilde{\mathcal{E}}/\tilde{n} = \mathcal{E}/(\tilde{n}E_B/a^3)$ for three-dimensional Rabi-coupled bosons in the small Rabi frequency regime

$$\begin{aligned} \frac{\widetilde{\mathcal{E}}}{\widetilde{n}} &= \pi(1+\epsilon)\widetilde{n}-\widetilde{\omega}_R \\ &+ \frac{32\sqrt{2\pi}}{15}(1+\epsilon)^{5/2}\widetilde{n}^{3/2}\Big[1+\frac{5}{4\pi}\frac{\widetilde{\omega}_R}{(1+\epsilon)\widetilde{n}}\Big] \\ &+ \frac{32\sqrt{2\pi}}{15}(1-\epsilon)^{5/2}\widetilde{n}^{3/2}\Big[1+\frac{5}{8\pi}\frac{(3-\epsilon)\widetilde{\omega}_R}{(1-\epsilon^2)\widetilde{n}}\Big]. \end{aligned} \tag{2.41}$$

The first line corresponds to the mean-field contribution obtained from Eq. (2.12). The second line is calculated from Eq. (2.31). We emphasize that using Eq. (2.31) to obtain directly the energy, the result is not dependent on the Rabi-coupling. This procedure gives rise to the third term in the energy given by Eq. 14 in Ref. [115]. However, here we use a different approximation. We first apply the small Rabi-frequency approximation in Eq. (2.31) and then we calculate the energy, as a result we have the second line in Eq. (2.41). The last line in Eq. (2.41) is calculated from Eq. (2.30). The second term here also does not coincide with the fifth term of Eq. 14 in Ref. [115], although we use two regularization methods to solve the integral with the same result in both cases. In other words, our results do not entirely coincide with those obtained in Ref. [115].

Now, regarding the droplet phase we have that if $\epsilon \lesssim -1$ the contribution proportional to $(1+\epsilon)^{5/2}$ becomes imaginary inducing dissipation. However if the density is not too large such hat this dissipative contribution is small enough, we can neglect it. In that case the resulting energy per particle has the characteristic attraction-repulsion competition typical of a droplet and we obtain the energy of Rabi-coupled bosonic droplets given by

$$\frac{\widetilde{\mathcal{E}}_D}{\widetilde{n}} = -\pi(|\epsilon|-1)\widetilde{n} - \widetilde{\omega}_R + \frac{32\sqrt{2\pi}}{15}(1+|\epsilon|)^{5/2}\widetilde{n}^{3/2}\Big[1 - \frac{5}{8\pi}\frac{(3+|\epsilon|)\widetilde{\omega}_R}{(|\epsilon|^2-1)\widetilde{n}}\Big]. \tag{2.42}$$

We can see how the Rabi-frequency contributes with extra attraction to the usual droplet. This attraction appears both at mean-field level and considering the Gaussian corrections.

The two-dimensional droplet

Now we discuss the two-dimensional case. Using the energy in the mean-field approximation obtained from Eq. (2.12), and the grand-canonical potential from Eqs. (2.37), and (2.38), the homogeneous ground-state energy density $\mathcal{E} = E/L^2$ can be read as [55]

$$\begin{aligned}\mathcal{E} &= \frac{1}{4}g_+n^2 - \hbar\omega_R n + \frac{m}{32\pi\hbar^2}g_+^2n^2\ln\left(\frac{\sqrt{e}mg_+n}{2\hbar^2\kappa^2}\right) \\ &+ \frac{m}{32\pi\hbar^2}g_-^2n^2\ln\left[\frac{m(g_-n+4\hbar\omega_R)}{2\hbar^2\kappa^2e^{-\delta/2}}\right],\end{aligned} \tag{2.43}$$

with $g_\pm = g(1\pm\epsilon)$, $\delta = (1-\sqrt{B}/A)/(1+\sqrt{B}/A)$, $2A = g_-n + 4\hbar\omega_R$, and $B = 2\hbar\omega_R(g_-n + 2\hbar\omega_R)$. Now, for simplicity, we set $m = \hbar = 1$, and we consider weakly attractive inter- and weakly repulsive intraspecies interactions, where $1/a_{\uparrow\downarrow} \ll \sqrt{n} \ll 1/a$ [24]. We find that a self-bound droplet structure is present, however, it can be unstable. Following the lines of Ref. [24], we introduce a new momentum cutoff κ_c including the set of coupling constants defined as $\tilde{g} = 4\pi/\ln[4e^{-2\gamma}/(a^2\kappa_c^2)]$, and $\tilde{g}_{\uparrow\downarrow} = 4\pi/\ln[4e^{-2\gamma}/(a_{\uparrow\downarrow}^2\kappa_c^2)]$. We choose $\kappa_c^2 = 4e^{-2\gamma}/(a_{\uparrow\downarrow}a)$ such that $\tilde{g}_{\uparrow\downarrow}^2 = \tilde{g}^2$. Provided that κ_c/κ is not exponentially large, g

and $\tilde{g}$ are equivalent. Thus from Eq. (2.43) the energy of a droplet is

$$\frac{\mathcal{E}_D}{n} = -\omega_R + \frac{g^2 n}{8\pi} \ln\left(\frac{gn + 2\omega_R}{\tilde{\epsilon}_c e^{-\tilde{\delta}/2}}\right), \tag{2.44}$$

where $\tilde{\delta} = (1 - \sqrt{\tilde{B}/\tilde{A}})/(1 + \sqrt{\tilde{B}/\tilde{A}})$, $\tilde{A} = gn + 2\omega_R$, and $\tilde{B} = 4\omega_R(gn + \omega_R)$.

The one-dimensional droplet

Now we discuss the two-dimensional case. Using the energy in the mean-field approximation obtained from Eq. (2.12), and the grand-canonical potential from Eqs. (2.33), and (2.34), the homogeneous ground-state energy density $\mathcal{E} = E/L^2$ can be read as

$$\begin{aligned}\mathcal{E} &= \frac{1}{4}g_+ n^2 - \hbar\omega_R n - \frac{1}{3\pi}\left(\frac{m}{2\hbar^2}\right)^{1/2}(g_+ n)^{3/2}\left(1 + \frac{3\hbar\omega_R}{g_+ n}\right) \\ &- \frac{1}{3\pi}\left(\frac{m}{2\hbar^2}\right)^{1/2}(g_- n)^{3/2}\left\{1 + \frac{3\hbar\omega_R}{g_- n}\left[\frac{g_-}{g_+} + \frac{1}{2}\ln\left(\frac{\hbar^2\kappa^2 e^4}{32 m g_- n}\right)\right]\right\}. \end{aligned} \tag{2.45}$$

In analogy with the $3d$ case and unlike reference [55], we first apply the small Rabi-frequency approximation in Eq. (2.34) and then we calculate the energy, and as a result we have the last term inside the parentheses in Eq. (2.45).

Now, we focus on the regime of repulsive intraspecies and attractive interspecies interactions with $|\epsilon| \equiv g_{12}/g \to 1^-$ [24]. By using $g = 2\hbar^2/m|a|$, $g_{12} = -2\hbar^2/m|a_{\uparrow\downarrow}|$ [126], and by taking $E_B = \hbar^2/m|a|^2$ as the energy unit, we define $\bar{n} = n|a|$, $\bar{\omega}_R = \hbar\omega_R/E_B$, and $\bar{\kappa} = \kappa/E_B$. Thus we get the scaled energy per particle of ultradilute and uniform Rabi-coupled droplets $\bar{\mathcal{E}}_D/\bar{n} = \mathcal{E}_D/(\bar{n}E_B/|a^{1D}|)$ as

$$\frac{\bar{\mathcal{E}}_D}{\bar{n}} = \frac{1}{2}\epsilon_- \bar{n} - \bar{\omega}_R - \frac{4\sqrt{2}}{3\pi}\bar{n}^{1/2} - \frac{2\sqrt{2}}{\pi}\frac{\bar{\omega}_R}{\epsilon_- \bar{n}^{1/2}}, \tag{2.46}$$

where $\epsilon_- = 1 - |\epsilon| \to 0$. In this regime, we find that $4\epsilon_-^{-1} \gg \ln\left(\bar{\kappa}/4\bar{n}\right)$. So, we check that the logarithmic contribution of energy in Eq. (2.45) does not affect the results, and hence it is neglected. Regarding this logarithmic term, we also consider the scaled energy per particle in a general context. We find that for $0 < \epsilon < 1$, the effect of $\bar{\kappa}$ is not relevant either. We confirm our results by using $3 \cdot 10^{-1} \leq \bar{\kappa} \leq 5 \cdot 10^3$. Of course, one would expect the result to be independent of the scale parameter. This issue could be further analyzed using the renormalization group which is beyond the scope of this work.

By minimizing Eq. (2.46) with respect to density, we find two possible physical solutions which are written as

$$\bar{n}_j = \frac{128}{81\pi^2\epsilon_-^2}\left[\cos\left[\frac{1}{3}\cos^{-1}\theta(\bar{\omega}_R,|\epsilon|) - \frac{2\pi}{3}j\right] + \frac{1}{2}\right]^2, \tag{2.47}$$

where $\theta = 1 - 729\pi^2\bar{\omega}_R\epsilon_-/128$, and $j = 0, 1$. For $j = 0$ we have the equilibrium density, hereafter called $\bar{n}_0$, while for $j = 1$ the solution is a local maximum. From $\bar{n}_0$ we find a stable mixture for $0 < \bar{\omega}_R(1 - |\epsilon|) \leq 256/(729\pi^2)$ [55]. We also obtain the spinodal density region of the mixture $\bar{n}^{\mathrm{sp}}$, which is defined by the condition $\partial^2\bar{\mathcal{E}}/\partial\bar{n}^2 = 0$. This spinodal density has the same form of Eq. (2.47), provided that $\epsilon_- \to 4\epsilon_-/3$ and $\omega_R \to 4\omega_R/9$. So, the mixture is thus metastable for $\bar{n}^{\mathrm{sp}} < \bar{n} < \bar{n}_0$.

2.3.2 Gaussian fluctuations including the nonuniversal corrections to the interactions

Now, in addition to having the same intra-species couplings, we have also considered the simplified scenario where the intra-species nonuniversal effects to the interactions are equal, such that $g_{11}^{(2)} = g_{22}^{(2)} = g^{(2)}$. In analogy with the subsection above we have that the grand potential of the Gaussian fluctuations Ω_{GF} is provided by [82]

$$\Omega_{\mathrm{GF}} = \frac{1}{2\beta}\sum_{k>0}\sum_{n=-\infty}^{+\infty}\ln\det[\mathbb{G}^{-1}(k,\omega_n)], \tag{2.48}$$

with the bosonic Matsubara's frequencies $\omega_n = 2\pi n/(\hbar\beta)$, and the 4×4 inverse fluctuation propagator $\mathbb{G}^{-1}$ given as

$$\mathbb{G}^{-1} = \begin{pmatrix} \mathbf{G}_{11}^{-1} & \mathbf{G}_{12}^{-1} \\ \mathbf{G}_{12}^{-1} & \mathbf{G}_{22}^{-1} \end{pmatrix}, \tag{2.49}$$

with the symmetric 2×2 matrices

$$\mathbf{G}_{11}^{-1} = \begin{pmatrix} -i\hbar\omega_n + f_1(k) & \frac{1}{2}(g^{(0)} + g^{(2)}k^2)\phi^2 \\ \frac{1}{2}(g^{(0)} + g^{(2)}k^2)\phi^2 & i\hbar\omega_n + f_1(k) \end{pmatrix}, \tag{2.50}$$

where $f_1(k) = \varepsilon_k + \frac{1}{2}(2g^{(0)} + g_{12}^{(0)} + g^{(2)}k^2)\phi^2 - \mu$, with the free-particle energy $\varepsilon_k = \hbar^2 k^2/2m$, $\mathbf{G}_{22}^{-1} = \mathbf{G}_{11}^{-1}(1 \leftrightarrow 2)$, and

$$\mathbf{G}_{12}^{-1} = \begin{pmatrix} \frac{1}{2}(g_{12}^{(0)} + g_{12}^{(2)}k^2)\phi^2 - \hbar\omega_R & \frac{1}{2}(g_{12}^{(0)} + g_{12}^{(2)}k^2)\phi^2 \\ \\ \frac{1}{2}(g_{12}^{(0)} + g_{12}^{(2)}k^2)\phi^2 & \frac{1}{2}(g_{12}^{(0)} + g_{12}^{(2)}k^2)\phi^2 - \hbar\omega_R \end{pmatrix}. \tag{2.51}$$

By solving the determinant of the inverse propagator we get

$$\Omega_{\mathrm{GF}} = \frac{1}{2\beta} \sum_{\substack{k>0 \\ n=-\infty}}^{+\infty} \ln\left[(\hbar^2\omega_n^2 + E_+^2)(\hbar^2\omega_n^2 + E_-^2)\right], \tag{2.52}$$

with the Bogoliubov spectra given as

$$E_+ = \sqrt{(1 + \mu_R\delta_+)\varepsilon_k^2 + 2\mu_R\varepsilon_k}, \tag{2.53}$$

and

$$E_- = \sqrt{(1 + \mu_R\delta_-)\varepsilon_k^2 + 2A\varepsilon_k + B} \tag{2.54}$$

with $A = 2\hbar\omega_R + \mu_R(\lambda + \hbar\omega_R\delta_-)$, $B = 4\hbar\omega_R(\hbar\omega_R + \lambda\mu_R)$,

$$\delta_\pm = \frac{4m}{\hbar^2}\Big(\frac{g^{(2)} \pm g_{12}^{(2)}}{g^{(0)} + g_{12}^{(0)}}\Big), \qquad \lambda = \frac{g^{(0)} - g_{12}^{(0)}}{g^{(0)} + g_{12}^{(0)}}. \tag{2.55}$$

The sum over the bosonic Matsubara's frequencies given by Eq. (2.23) has two contributions, one at zero-temperature and the other at finite-temperature [51, 82, 90]. We neglect the contribution at finite temperature considering only the zero-temperature term which is given by

$$\Omega_{\mathrm{GF}} = \frac{1}{2}\sum_{k,\pm} E_\pm(k), \tag{2.56}$$

which in turn in the continuum limit $\sum_k \to V\int d^3k/(2\pi)^3$, can be read as follows

$$\frac{\Omega_{\mathrm{GF}}}{V} = \frac{\Omega_{\mathrm{GF}}^+}{V} + \frac{\Omega_{\mathrm{GF}}^-}{V} \tag{2.57}$$

with the ultraviolet divergent integrals

$$\frac{\Omega^{+}_{\mathrm{GF}}}{V} = \int_0^\infty \frac{dk}{4\pi^2} k^2 E_+, \tag{2.58}$$

and

$$\frac{\Omega^{-}_{\mathrm{GF}}}{V} = \int_0^\infty \frac{dk}{4\pi^2} k^2 E_-. \tag{2.59}$$

In addition the second integral has not a closed form. Therefore in order to get some analytical results and to know some insights into the underlying physics, we consider the limit of weak Rabi frequency, such that, $\omega_R \ll \mu/\hbar$ [115, 119]. So by expanding up the Bogoliubov spectra to first order in the Rabi frequency, we get

$$E_+ = [\varepsilon_k^2(1+\delta_+\mu) + 2\mu\varepsilon_k]^{1/2} + \frac{\varepsilon_k(2+\varepsilon_k\delta_+)\hbar\omega_R}{2[\varepsilon_k^2(1+\delta_+\mu)+2\mu\varepsilon_k]^{1/2}} + \mathcal{O}\big((\frac{\hbar\omega_R}{\mu})^2\big), \tag{2.60}$$

and

$$\begin{aligned} E_- &= [\varepsilon_k^2(1+\delta_-\mu) + 2\lambda\mu\varepsilon_k]^{1/2} \\ &+ \frac{[\varepsilon_k^2\delta_- + 2\varepsilon_k(2+\lambda+\mu\delta_-) + 4\lambda\mu]\hbar\omega_R}{2[\varepsilon_k^2(1+\delta_-\mu)+2\lambda\mu\varepsilon_k]^{1/2}} + \mathcal{O}\Big(\Big(\frac{\hbar\omega_R}{\mu}\Big)^2\Big). \end{aligned} \tag{2.61}$$

The new ultraviolet divergent integrals are solved by means of dimensional regularization [55, 82], and the resulting two branches of the grand potential are

$$\frac{\Omega^{+}_{\mathrm{GF}}}{V} = \frac{8}{15\pi^2}\Big(\frac{m}{\hbar^2}\Big)^{3/2} \frac{\mu^{5/2}}{(1+\delta_+\mu)^2}\Big[1 + \frac{1}{2}\Big(\frac{5+\delta_+\mu}{1+\delta_+\mu}\Big)\frac{\hbar\omega_R}{\mu}\Big], \tag{2.62}$$

obtained from Eq. (2.60), and

$$\begin{aligned} \frac{\Omega^{-}_{\mathrm{GF}}}{V} &= \frac{8}{15\pi^2}\Big(\frac{m}{\hbar^2}\Big)^{3/2} \frac{\lambda^{5/2}\mu^{5/2}}{(1+\delta_-\mu)^2}\Big[1 + \frac{1}{4\lambda(1+\delta_-\mu)} \\ &\times \big[2\lambda(5+\delta_-\mu) + 5[1-(\delta_-\mu)^2]\big]\frac{\hbar\omega_R}{\mu}\Big]. \end{aligned} \tag{2.63}$$

obtained from Eq. (2.61). We stress that the first integral in Eq. (2.57) can be solved directly, for any value of Rabi frequency, by means of dimensional regularization

[50, 82, 91, 92], resulting

$$\frac{\Omega_{\rm GF}^{+}}{V} = \frac{8}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{\mu_R^{5/2}}{(1+\delta_+\mu_R)^2}, \tag{2.64}$$

and the grand potential in Eq. (2.62) can be also obtained directly from Eq. (2.64) in the limit of small Rabi coupling. We stress that in absence of non-universal corrections Eq. (2.64) was considered in [115]. In this reference the grand potential was used directly to obtain the third term in the energy given by Eq. 14, which is independent of the Rabi coupling. However the two last contributions in such a energy are obtained in the approximation of weak Rabi frequency (see also [55] for a one-dimensional version of this issue with the same consideration). Here, we calculate the energy from the two branches of the grand potential in the limit of small Rabi coupling given by Eqs. (2.62) and (2.63). In this way we show that in absence of the non-universal contribution our results for the energy do not completely match from those obtained in [115].

Now we consider $E_B = \hbar^2/ma^2$ as energy unit, the Rabi-frequency $\widetilde{\omega}_R E_B = \hbar\omega_R$, $\widetilde{n} = na^3$, the energy density $\mathcal{E} = E/V$, the ratios $\epsilon = a_{12}/a$, $\gamma = r/a$, and $\gamma_{12} = r_{12}/a$. This leads to the total scaled energy density $\widetilde{\mathcal{E}} = \mathcal{E}/(E_B/a^3)$ for nonuniversal Rabi-coupled interacting bosonic gases in the small Rabi frequency regime

$$\begin{aligned}
\widetilde{\mathcal{E}} &= \pi(1+\epsilon)\widetilde{n}^2 - \widetilde{\omega}_R\widetilde{n} \\
&+ \frac{32\sqrt{2\pi}}{15}\frac{[(1+\epsilon)\widetilde{n}]^{5/2}}{(1-h_{\rm fr}^{+}\widetilde{n})^2}\left[1+\frac{\widetilde{\omega}_R}{4\pi(1+\epsilon)\widetilde{n}}\left[\frac{5-h_{\rm fr}^{+}\widetilde{n}}{1-h_{\rm fr}^{+}\widetilde{n}}\right]\right] \\
&+ \frac{32\sqrt{2\pi}}{15}\frac{[(1-\epsilon)\widetilde{n}]^{5/2}}{(1+h_{\rm fr}^{-}\widetilde{n})^2}\left\{1+\frac{\widetilde{\omega}_R}{8\pi(1-\epsilon)\widetilde{n}}\frac{1}{(1+h_{\rm fr}^{-}\widetilde{n})}\right. \\
&\times \left.\left[2\left(\frac{1-\epsilon}{1+\epsilon}\right)(5+h_{\rm fr}^{-}\widetilde{n})+5[1-(h_{\rm fr}^{-}\widetilde{n})^2]\right]\right\},
\end{aligned} \tag{2.65}$$

where $h_{\rm fr}^{\pm} = 4\pi(\gamma_{12}^3 \pm \gamma^3)/3$. We have included the mean-field energy density given by Eq. (2.12) in the first line. The second line is obtained from Eq. (2.62), and the last two from Eq. (2.63). By considering the couplings in Eqs. (2.2) and (2.3) it is necessary taking into account the change of variable $\gamma_{12}^3 \pm \gamma^3 \rightarrow \mp 3(\gamma \pm \epsilon^2\gamma_{12})$.

2.3.3 Nonuniversal droplet phase

The energy density in Eq. (2.65) is well-defined for $-1 < \epsilon \leq 1$, in correspondence with the prediction set by the mean-field analysis, as it was discussed at end of section 2.2.1. In absence of the Rabi coupling, the miscible phase, is achieved for $0 < \epsilon < 1$ [44, 45], at mean-field level. However the Rabi frequency allows such a region to be extended for $-1 < \epsilon < 0$, as we can see in Fig. 2.1. In Eq. (2.65) providing $\epsilon \leq -1$ the fluctuations sector becomes unstable in analogy with the unstable region in Fig. 2.1. However the configuration is also not stable providing $\epsilon > 1$, associated with the presence of the fluctuations, even if the energy density of the mean-field ground state is stable. Although the configuration is not stable for $\epsilon > 1$, and $\epsilon < -1$, we can do the following analysis. In the first instance we will analyze the mean field collapse region of the Bose-Bose mixture, i.e. when the interspecies attraction $g_{12}^{(0)} < 0$ becomes stronger than intraspecies repulsion $g^{(0)} > 0$, such that $\epsilon < -1$. It is clear that if $\epsilon \to -1^-$, the second line in the energy density given by Eq. (2.65) becomes imaginary, and it could be induce instability [23]. However if $\bar{n}$ is not too large such hat this contribution is small enough such that its effect is only dissipative, as a physically reasonable assumption we can neglect it [23, 115]. Under the above mentioned consideration, the system exhibits a liquidlike phase where Rabi-coupled Bose-Bose droplets with nonuniversal effects to the interactions emerge. The respective scaled energy density for this phase is given by

$$\begin{aligned}\widetilde{\mathcal{E}}_D &= \pi(1-|\epsilon|)\widetilde{n}^2 - \widetilde{\omega}_R\widetilde{n} + \frac{32\sqrt{2\pi}}{15}\frac{[(1+|\epsilon|)\widetilde{n}]^{5/2}}{(1+h_{\rm fr}^{-}\widetilde{n})^2} \\ &\times \left\{1 + \frac{\widetilde{\omega}_R}{8\pi(1+|\epsilon|)\widetilde{n}}\frac{1}{(1+h_{\rm fr}^{-}\widetilde{n})}\left[2\left(\frac{1+|\epsilon|}{1-|\epsilon|}\right)(5+h_{\rm fr}^{-}\widetilde{n})+5\right]\right\}. \qquad (2.66)\end{aligned}$$

In a attempt for fitting theoretical predictions and numerical results for conventional droplets [47], it is employed the approximation $|\epsilon| = 1$ only on the fluctuations sector. However, if we use $|\epsilon| = 1$ only on fluctuations of Eq. (2.66), the last term becomes divergent and we have not a stable ground-state. On the other hand, for $\epsilon \gtrsim 1$, and neglecting the imaginary contribution of Eq. (2.65), the resulting total real energy density is stable. However in this scenario the effect of repulsive Gaussian fluctuations is imperceptible regarding leading repulsive mean-field term. Therefore these are not relevant and can be neglected.

In Fig. 2.2 we plot the shifted energy per particle $\widetilde{\mathcal{E}}_D/\widetilde{n} + \omega_R$ obtained from Eq.

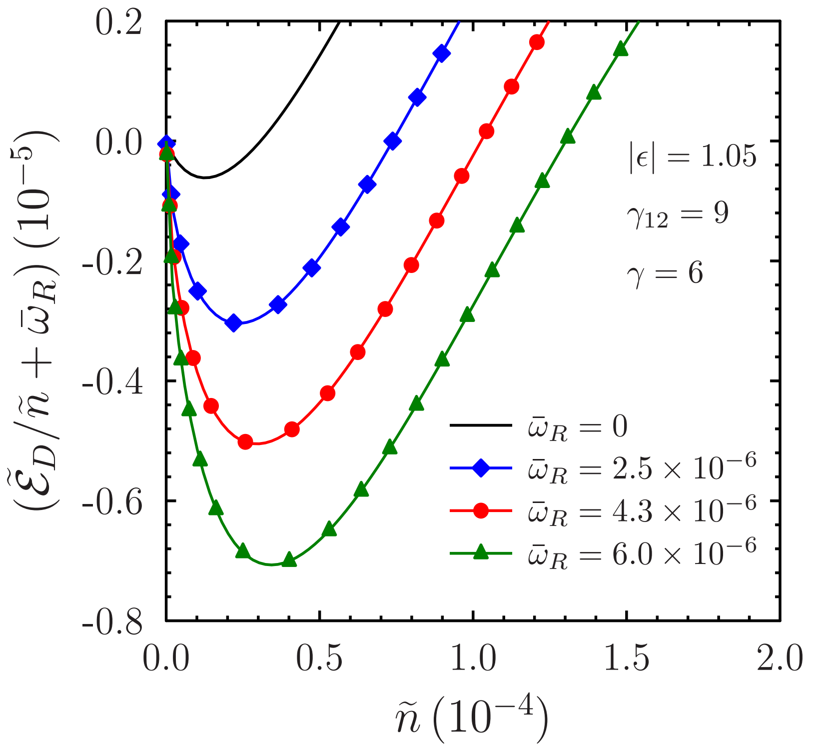

Figure 2.2: Shifted energy per particle $\tilde{\mathcal{E}}_D/\tilde{n} + \omega_R$ for droplets in Rabi-coupled Bose-Bose gases with nonuniversal corrections to the interactions as function of the scaled density, Eq. (2.66). We consider the ratio $\epsilon \lesssim -1$ such that $|\epsilon| = 1.05$ between attractive inter-species and repulsive intra-species. We set $\gamma_{12} = 9$ and $\gamma = 6$. We consider $\bar{\omega}_R = 0$ (solid black line), $\bar{\omega}_R = 2.5 \times 10^{-6}$ (blue diamonds), $\bar{\omega}_R = 4.3 \times 10^{-6}$ (red circles), and $\bar{\omega}_R = 6.0 \times 10^{-6}$ (green triangles).

(2.66). We set $|\epsilon| = 1.05$, $\gamma_{12} = 6$, and $\gamma = 9$ with the scaled Rabi frequencies $\bar{\omega}_R = 0, 2.5 \times 10^{-6}, 4.3 \times 10^{-6}$, and 6.0×10^{-6}. Taking into account ultracold ^{39}K atoms these Rabi frequencies correspond to $\bar{\omega}_R \sim 0, 40.6, 69.8$, and 97.4 Hz, respectively. The behavior described above is also obtained for frequencies up to $\bar{\omega}_R = 22 \times 10^{-5}$ ($\sim$ 3572.87 Hz for atoms of ^{39}K). Here we have considered the couplings in Eqs. (2.4), and (2.5). This can be understood since taking into account only the mean-field energy per particle the attraction causes the condensate to collapse, therefore the strong attraction lead us to consider the nonuniversal corrections to the attractive interactions, such that $r_{12} \gg a_{12}$, as a relevant contribution. However as repulsion is very close to attraction, and with the aim of obtaining a more complete overview of the effects of the nonuniversal corrections to the interactions we also include the nonuniversal correction to the repulsion such that $r \gg a$. Experimental values of the s-wave scattering length and the nonuniversal corrections to the interactions as a function of the external magnetic field in ultracold ^{39}K atoms show that it is possible to satisfy the condition $r \gg a$ [48, 97]. In addition, if we use the couplings (2.2) and (2.3), the nonuniversal effects to the interactions on the droplet energy per particle are not perceptible. Droplets with $\bar{\omega}_R = 0$ and nonuniversal corrections to the interactions were recently considered in Ref. [50]. In such a work neglecting the nonuniversal corrections to the repulsive interactions, and using the nonuniversal contribution to the attractive interactions as a fitting parameter it is obtained a good agreement between the theoretical predictions and some diffusion Monte Carlo calculations (DMC) [47]. In Fig. 2.2, and considering $a \sim 100$Å we have densities of order $n \sim 10^{14}$atoms/cm^3. Our results also apply for densities of order 10^{13}atoms/cm^3, experimentally obtained for conventional droplets [25, 26]. The increase in the driving of the population transfer between the two atomic levels by means of the increase of the frequency values allows us to evidence an increasing into effective attraction of the system, both at mean-field level and in the Gaussian fluctuations since $|\epsilon| > 1$. This leads to have a greater number of atoms in the ground-state compared to the no presence of the Rabi coupling.

In Fig. 2.3 (a)-(b) we plot the phase diagram for the density of the Rabi-coupled droplets with nonuniversal corrections to the interactions and the respective energy per particle as a function of the ratio $|\epsilon|$. The nonuniversal corrections to the attraction and to the repulsion are fixed as $\gamma_{12} = 9$, and $\gamma_{12} = 6$, respectively. We set the values of the Rabi frequencies $\bar{\omega}_R = 6.16 \times 10^{-6}$ (~ 100 Hz for atoms of ^{39}K), and $\bar{\omega}_R = 4.93 \times 10^{-6}$ (~ 80 Hz for atoms of ^{39}K). The red line represents the critical value of $|\epsilon|$ with $|\epsilon_c| = 1.083$, such that providing $|\epsilon| > |\epsilon_c|$ the droplet collapses. In both Figs. 2.3 (a)-(b) we have not monotonically growing functions of the ratio $|\epsilon|$. For values greater than $|\epsilon| \sim 1.04$ the behavior is an expected consequence when the leading contribution, the attraction, increases. In other words, we can see how increasing the atomic attraction the density of the droplet is increasingly and eventually this becomes unstable. Such a behavior is also present for different values of the frequency. However, it is worth mentioning that due to the asymptotic behavior for $|\epsilon| \to 1$ related to the divergence in the fluctuation sector of Eq. (2.66), we also have an increasing both in density and in the energy per particle for $|\epsilon| \lesssim 1.04$. Similar results with the same threshold for $|\epsilon|$ have been also obtained for frequencies up to $\bar{\omega}_R = 22 \times 10^{-5}$ (~ 3572.87 Hz for atoms of ^{39}K). In Fig. 2.3 (c) we include the phase diagram for the nonuniversal corrections to the interactions encoded in $h^{-}_{\mathrm{fr}} > 0$ as a function of $|\epsilon|$ for a frequency of $\bar{\omega}_R = 7.39 \times 10^{-6}$ (~ 120 Hz for atoms of ^{39}K). We can see how fixing both the

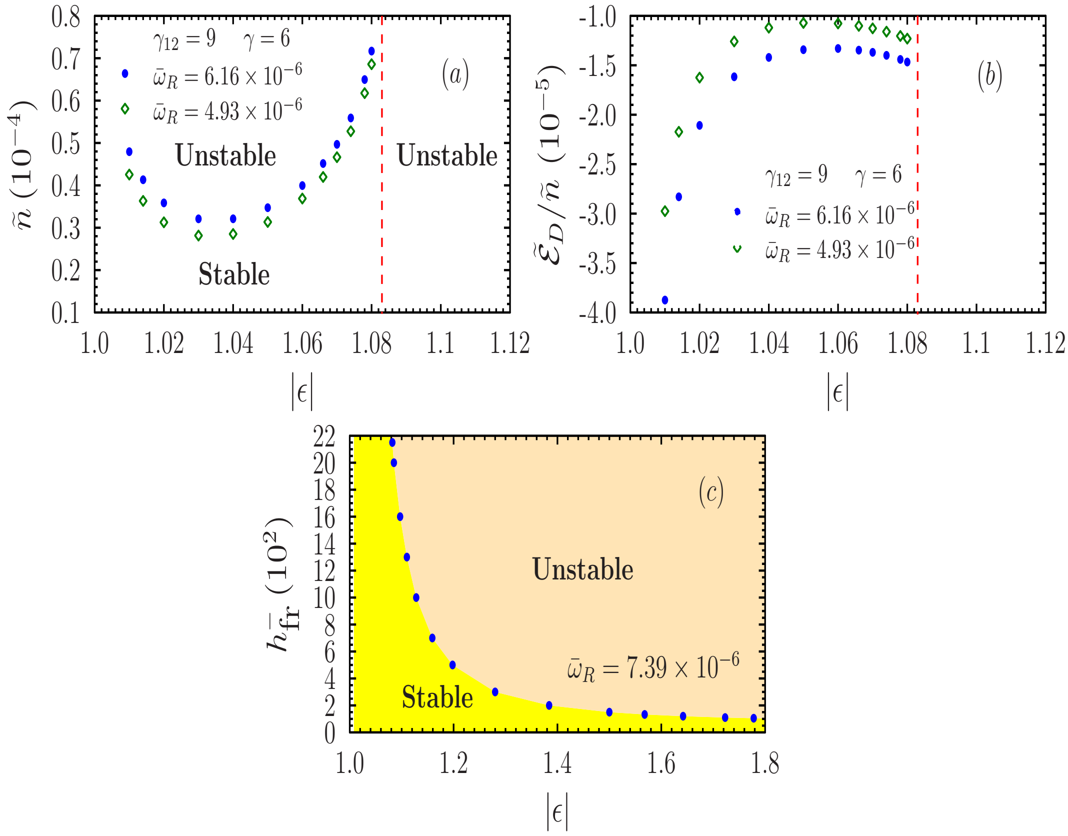

Figure 2.3: (a)-(b) Phase diagram for the density of the Rabi-coupled droplets with nonuniversal corrections to the interactions and the respective energy per particle as a function of the ratio $|\epsilon|$. The nonuniversal correction to the attractions and to the repulsions are $\gamma_{12} = 9$, and $\gamma = 6$, respectively. We set the values of the Rabi frequency $\bar{\omega}_R$ as 6.16×10^{-6}, and 4.93×10^{-6}. The dashed red line represents the threshold value for $|\epsilon|$ as $|\epsilon_c| = 1.083$. (c) Phase diagram for the nonuniversal corrections to the interactions encoded in $h^{-}_{\mathrm{fr}} > 0$ as a function of $|\epsilon|$ for a frequency of $\bar{\omega}_R = 7.39 \times 10^{-6}$.

Rabi frequency and the ratio $|\epsilon|$, and since h^{-}_{fr} increases, the attraction exceeds of repulsion and the effective contribution given by the nonuniversal corrections to the interactions allows an increasing in the equilibrium density. However, for sufficiently large values of h^{-}_{fr}, inelastic collisions decrease the number of atoms that can be accommodated in a stable ground-state until we no longer find a minimum in the energy density. The system exhibits an instability and there is not a self-bound state formation, as it was proposed recently in droplets with nonuniversal corrections to the interactions in Bose-Bose mixtures without Rabi coupling [50]. We can also see how the threshold for the instability established by $|\epsilon|$ is smaller as the h^{-}_{fr} increases, as it is expected. This can be understood due to the fact that the leading contribution is attractive.

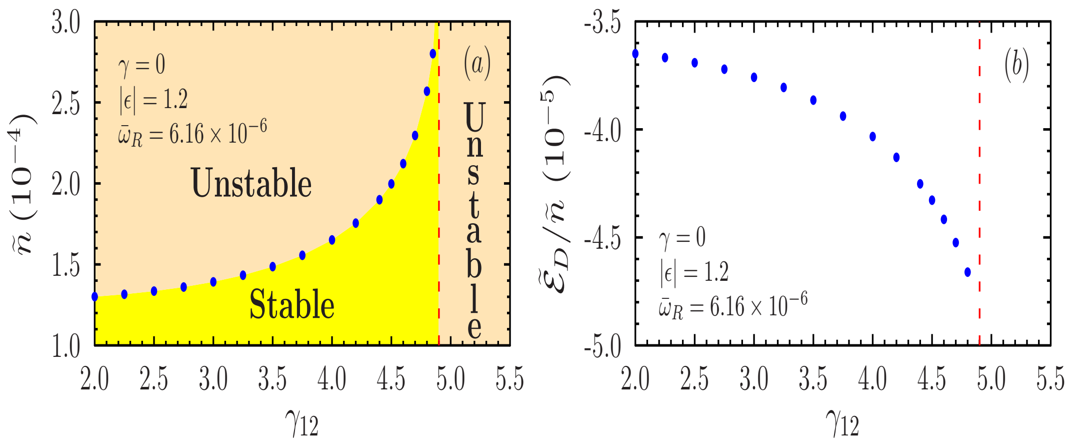

Figure 2.4: (a) Phase diagram for the density, and (b) energy per particle of the Rabi-coupled droplets with nonuniversal corrections to the interactions as function of the nonuniversal effects to the attractive interactions γ_{12}. The nonuniversal corrections to the repulsive interactions are fixed by $\gamma = 0$. We set$|\epsilon| = 1.2$ and the Rabi coupling $\bar{\omega}_R = 6.16 \times 10^{-6}$. The dashed red line represents the threshold value for $\gamma_{12}^c = 4.901$.

In Fig. 2.4 we plot the phase diagram for the density and the energy per particle for Rabi-coupled droplets with nonuniversal corrections to the interactions as function of the nonuniversal effects of the attractive interactions γ_{12}. The nonuniversal corrections to the repulsions are fixed by $\gamma = 0$. We set $|\epsilon| = 1.2$ and the Rabi coupling $\bar{\omega}_R = 6.16 \times 10^{-6}$ ($\sim$ 100 Hz for atoms of ^{39}K). The dashed red line represents the threshold values of γ_{12} with $\gamma_{12}^c = 4.901$. In other words for values greater than γ_{12}^c, the droplet becomes unstable by collapse. In Fig. 2.4 (a) fixing the effective attraction with constant values of $|\epsilon|$, and γ_{12} and increasing the density we get an increase in the droplet energy per particle Fig. 2.4 (b), until reaching a point where it is no longer possible to maintain a stable ground state. The effective attraction dominates the kinetic energy, so the droplet shrinks, but once a threshold in $\bar{n}$ is reached the droplet becomes so attractive that it is destroyed by inelastic collisions. As a result of it, there is not a minimum in energy per particle. This effect is also observed when the increase of the nonuniversal correction to the attraction increases the density. The droplet is more attractive and eventually this becomes unstable beyond γ_{12}^c. These results are equivalent to that presented in the Fig 2.3 (a)-(b), for values not close to the asymptote $|\epsilon| \to 1$. This behavior has been also obtained for frequencies up to $\bar{\omega}_R = 22 \times 10^{-5}$ ($\sim$ 3572.87 Hz for atoms of ^{39}K).

2.4 Summary and outlook

By considering an effective quantum field theory in the formalism of the path integrals up Gaussian level, we derive a closed expression for the zero-temperature equation of state for three-dimensional ultracold Rabi-coupled Bose-Bose mixtures of alkali-metal atoms with nonuniversal corrections to the interactions in the regime of weakly Rabi frequency. The ultraviolet divergences associated to both gapless and gapped elementary excitations in the Bogoliubov spectra are removed through dimensional regularization. We stress and focus on the case where inter-species interactions are weakly attractive and subtly higher than repulsive intra-species. Our results show that in this regime such mixtures manifest the stable formation of a liquidlike phase or a nonuniversal Rabi-coupled Bose-Bose droplet. Here the nonuniversal corrections to the interactions act as an additional tool to tune the stability properties of Bose-Bose Rabi-coupled droplets. Through phase diagrams in which the Rabi coupling is fixed and for suitable values of the ratio between the inter-species scattering length and the intra-species scattering lengths or the nonuniversal contribution to the interactions we establish some conditions under which the stable droplet formation can be achieved.

Due to the remarkable progress in the droplet phase research, it would be interesting to extend the present study to one and two dimensions [55], including dimensional crossovers [127]. In particular, in the one-dimensional model a more elaborate regularization process might be required for solve the ultraviolet divergence of the integrals [55]. Another extension of the present work could be related to the numerical study by means of quantum Monte Carlo techniques [47, 48]. Given the experimental relevance of trapping potentials it would be also interesting to consider, for example, harmonic traps to study the droplets obtained in the present work. Our theoretical predictions could stimulate experimental breakthroughs taking into account the density values considered. A promising candidate to the experimental observation of a nonuniversal Rabi-coupled droplet is the gas of ^{39}K atoms [118], by considering the second and third lowest Zeeman states of the lowest manifold for this atoms, i.e. $|F = 1, m_F = -1\rangle$, and $|F = 1, m_F = 0\rangle$. At a magnetic field $\sim 56.830(1)$G with the respective scattering lengths $a \sim 33.4a_0$, and $a_{12} \sim -53.2a_0$, where a_0 is the Bohr radius. Values of small Rabi frequency can be obtained below 6kHz [118], and some experimental values for $a, a_{12} \ll r, r_{12}$ are considered in [48, 97].

Chapter 3

Droplets in two coupled dipolar Bose-Einstein condensates

Following some of the ideas developed in previous chapters we extend our study to consider the dipole-dipole interactions in three-dimensional ultracold Bose-Bose gases. By considering an effective quantum field theory we derive the leading Gaussian zero-temperature corrections (or the dipolar-LHY corrections) and the Gaussian finite-temperature corrections to the equation of state of ultracold interacting dipolar Bose-Bose gases. In order to obtain closed analytical expressions, we consider a symmetric ground-state. At zero temperature we study some conditions under which the mean-field instability by collapse is avoided by the contribution arising from Gaussian fluctuations, driving thus to formation of a droplet. These conditions are established by the relation between the inter- and intraspecies contact couplings and the strength of the dipole-dipole interactions. In a local density approximation we introduce and address on an improved Gross-Pitaevskii equation (GPE) in which we analyze how the above mentioned parameters establish conditions under which the formation and stability of a self-bound miscible or immiscible droplet is favorable. We also obtain a GPE where a stable droplet formation could be achieved if the attractive interspecies and the repulsive intraspecies are equal. At low temperature taking into account the dependencies on the dipolar contribution but also the difference between intra- and inter-species coupling constants we calculate the thermal corrections to the grand-potential and to the GPEs above mentioned.

3.1 Introduction

For more than two decades the theoretical and experimental investigation of ultracold gases made of highly magnetic atoms has been extensive [40, 41, 42, 43], allowing thus the observation and study of unprecedented phenomena in which the anisotropic and long-range dipole-dipole interactions play a key role. In particular, in the last few years the subtle and highly nontrivial stabilization between the attractive mean-field energy and the repulsive energy coming from the fluctuations in mixtures of non-dipolar BECs has attracted an increasing interest [23], including also its respective extension to dipolar BECs. Due to this balance the mean-field collapse can be avoided allowing the emergence of a droplet phase, also including supersolid states (the supersolid state is characterized simultaneously for both a large superfluid fraction and the discrete translational symmetry), revealing thus the crucial role played by the fluctuations in dipolar BECs [33, 34, 35, 36, 37, 38, 39, 70, 71, 72, 73, 128, 129]. More recently, a quantum-Monte-Carlo-based density functional at zero temperature has been used to describe the droplet formation and the BEC-supersolid transition in ^{162}Dy atoms [130]. In this approximation the dipolar LHY term is substituted by the correlation energy evaluated with the quantum Monte Carlo method. The results reproduce the experimental value of the critical number of atoms required in the droplet formation. On the other hand, since the first observation of droplets and supersolid states of ultracold dipolar atoms, a huge progress has been made in understanding the zero-temperature phase diagram and low-energy excitations of these systems. However little is known regarding the finite-temperature effects on their properties, and this knowledge is relevant to the supersolids formation by cooling through direct evaporation [43, 131]. Usually to achieve a dipolar supersolid state, the starting point is an unmodulated BEC, then it is quenched the strength of the interatomic interactions to a value that favors a density-modulated state. In this production scheme, the superfluidity of the supersolid comes from the initial condensate. However, a dipolar supersolid can also be reached by direct evaporation from a thermal gas with fixed interactions. As it is known a thermal gas (non-condensed) lacks coherence and modulation, in that sense, both properties must emerge during the evaporative formation process. So far the understanding of the dipolar supersolidity is closely connected to the stabilization against the mean-field collapse by means of the Gaussian fluctuations, in that sense thermal fluctuations can also have effects on the phases of dipolar quantum gases, even below the condensation temperature. In a similar way an understanding of the effects of the temperature could be helpful for the design of evaporative cooling procedures in a controlled way. For instance, by solving an improved finite-temperature GPE describing a BEC confined in a tubular geometry has been shown as the temperature increasing can drive an instability from the superfluid to a supersolid phase

[132, 133]. The numerical results agree with the experiment values on ultracold Dy atoms, reproducing quantitatively the period and amplitude of the measured density modulations. Indeed, this indicates that the supersolid state can be best described including finite-temperature effects, which opens the door for exploring the unusual thermodynamics of dipolar quantum fluids. This instability can be understand analyzing the excitation spectrum of the condensate in the superfluid phase, where the local minimum of the dispersion at finite momenta supports the formation of a roton quasiparticle. Since the temperature increases, it generates a decreasing of the roton minimum and the density modulations becomes energetically more favorable. As a consequence a modulated phase eventually emerges. More recently has been achieved the production and stabilization of a mixture of ultracold dipolar Bose gases composed of the two lowest Zeeman states of ^{162}Dy atoms [134]. In these systems, a new interaction length scale arises due to interspecies interactions, thus opening a new branch in the study of quantum matter. For instance, it is possible to research the interplay between magnetic interactions, quantum fluctuations, and thermal effects.

On the other hand, few years ago it was numerically proposed the existence of self-bound dipolar droplets and supersolids in molecular BECs [135]. In this Ref. it was studied the many-body physics of NaRb molecular BECs with strong dipole-dipole interactions by means of an improved GPE. At experimental level, recent breakthroughs in the production of ultracold molecules have allowed the creation of 22000 bosonic NaCs molecules in their absolute rovibrational (rotational-vibrational) ground state at a temperature of $300(50)$ nK and a peak density of $1.0(4) \times 10^6\,\mathrm{m}^3$ [136]. A short time later and even more remarkable has been possible to achieve the observation of a very strongly dipolar condensate of NaCs molecules [137]. The strength of the dipolar interaction determined by the dipolar length in atoms of Dy has the value of $130.8a_0$, where a_0 is the Bohr radius. However in a NaCs molecule it is possible to obtain a very large dipolar length ranging from $1000a_0$ to $25000a_0$. Using quantum Monte Carlo simulations to study molecular BECs in the strongly dipolar regime have been obtained self-bound droplets, as well as their splitting into multiple droplets by confinement-induced frustration [138]. By means of the numerical study of a finite-temperature improved GPE has been found a good agreement with the experimental measurements for the condensate of dipolar NaCs molecules [139]. The ultracold dipolar molecules have been also studied using path-integral quantum Monte Carlo simulations [140], finding that for stronger interactions, the droplet continuously loses superfluidity and eventually it undergo a transition to a self-bound crystalline monolayer. This spontaneous formation is closed related to the long-range and anisotropic behaviour of the dipole-dipole interaction generated by microwave-dressing of rotational molecular states. Recently, the numeric solution of an improved GPE at zero temperature has shown that in a very strongly dipolar BEC with molecules of NaCs, it is possible to have a two- and a four-droplet metastable soliton, axially free along the polarization z direction [141]. A few weeks ago the experimental formation of self-bound droplets and droplet arrays in an ultracold gas of strongly dipolar NaCs molecules was reported [142]. Starting from a weakly interacting molecular BEC, microwave dressing fields are used to induce dipole-dipole interactions with controllable strength and anisotropy.

Taking into account the above we can see as the dipolar BECs at zero or finite temperature are excellent platforms for studying quantum effects at atomic level, and these are, at least in principle, a good approximation to study dipolar molecules. The rest of the chapter is organized as follows. In section 3.2, we introduce an effective-field theory in the path-integral formalism for three-dimensional interacting dipolar Bose-Bose gases. Then in section 3.3, we derive the mean-field grand-canonical potential and the grand-canonical potential from the Gaussian fluctuations, at zero temperature. In order to obtain closed analytical expressions we simplify the problem by considering a symmetric scenario. In this case and taking into account a local-density approximation we include two improved GPEs. From these GPEs we analyze some conditions for the existence of a stable droplet. In section 3.4 we study the finite-temperature corrections to the grand-potential. In section 3.5 we present a final discussion including some future perspectives of our results.

3.2 Model and preliminaries

We consider two-component bosonic gases with contact interactions plus dipole-dipole interactions in the path-integral formalism, see appendix A. For simplicity, we assume that the atomic masses of the two components are equal as in a Dy-Dy mixture [134, 143]. Including the chemical potential μ and confining the gas in a three-dimensional box of volume V the Lagrangian density for this system is $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}}$, where

$$\mathcal{L}_0 = \sum_{\alpha=1,2} \left[\psi_\alpha^*(\mathbf{r},\tau) \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2m} \nabla^2 - \mu_\alpha \right) \psi_\alpha(\mathbf{r},\tau) \right], \tag{3.1}$$

and

$$\mathcal{L}_{\text{int}} = \frac{1}{2}\sum_{\alpha,\sigma=1,2}\Big[g_{\alpha\sigma}|\psi_\alpha(\mathbf{r},\tau)|^2|\psi_\sigma(\mathbf{r},\tau)|^2 + \frac{1}{2}g^{dd}_{\alpha\sigma}\int d^3r d^3r'|\psi_\alpha(\mathbf{r},\tau)|^2 U^{dd}(\mathbf{r}-\mathbf{r}')|\psi_\sigma(\mathbf{r}',\tau)|^2\Big]. \tag{3.2}$$

The fields are considered at position $\mathbf{r}$ and imaginary time τ. Here, the strength of the interactions is expressed through the intra- and interspecies coupling constants $g_{\alpha\alpha} = 4\pi\hbar^2 a_{\alpha\alpha}/m$ and $g_{\alpha\sigma} = 4\pi\hbar^2 a_{\alpha\sigma}/m$, respectively. These in turn are related to the s-wave scattering lengths $a_{\alpha\alpha}$ and $a_{\alpha\sigma}$, respectively, such that $a_{\alpha\alpha}, a_{\alpha\sigma} > 0$ represent repulsion, and $a_{\alpha\alpha}, a_{\alpha\sigma} < 0$ attraction. We also have the intra- and interspecies coupling constants for the dipole-dipole interactions given by $g^{dd}_{\alpha\alpha} = \mu_0\bar{\mu}^2_\alpha/3 = 4\pi\hbar^2 a^{dd}_{\alpha\alpha}/m$, and $g^{dd}_{\alpha\sigma} = \mu_0\bar{\mu}_\alpha\bar{\mu}_\sigma/3 = 4\pi\hbar^2 a^{dd}_{\alpha\sigma}/m$ respectively. With μ_0 the permeability of vacuum and $\bar{\mu}_\alpha$ the magnetic dipole moments. This theory also applies for electric dipoles, where $\mu_0 \to \varepsilon_0^{-1}$ (the permittivity of vacuum), and $\bar{\mu} \to p_\alpha$ (the electric dipole moments). Finally,

$$U^{dd}(\mathbf{r}-\mathbf{r}') = \frac{3}{4\pi}\frac{1-3\cos^2\theta}{|\mathbf{r}-\mathbf{r}'|^3}. \tag{3.3}$$

Where θ is the angle between the direction of polarization and the relative position of the dipoles $\mathbf{r}$. It is well know that in contrasting with the isotropic short-range interaction the dipole-dipole interaction has a long-range character encoded in r^{-3}, and it is anisotropic which is reflected by the θ dependence. Whether $\theta = \pi/2$ we have $U^{dd}(\mathbf{r}) > 0$ and if $\theta = 0$ then $U^{dd}(\mathbf{r}) < 0$. So the dipole-dipole interaction is repulsive for particles sitting side by side, while this is attractive for dipoles in a 'head-to-tail' configuration with twice the strength of the previous case, i.e. $\left|U^{dd}(\theta = 0)\right| = 2\left|U^{dd}(\theta = \pi/2)\right|$ [40].

At zero temperature we assume the bosons condensate into the zero-momentum states. In order to perform a perturbative expansion we set $\psi_\alpha(\mathbf{r},\tau) = \phi_\alpha(\mathbf{r}) + \eta_\alpha(\mathbf{r},\tau)$. Where $\phi_\alpha(\mathbf{r}) \equiv \langle\psi_\alpha(\mathbf{r},\tau)\rangle$ [88], corresponds to the macroscopic condensate wave-function. The fluctuations around ψ_α are given by $\eta_\alpha(\mathbf{r},\tau)$ and these are orthogonal to the condensate of the same species [88, 89]. Since here the relative phases of the wave-functions do not play a role, we have $n_\alpha = |\phi_\alpha(\mathbf{r})|^2 = N_\alpha/V$, as the density of particles or condensate density in the mean-field approximation. Since $\phi_\alpha(\mathbf{r})$ describes the condensate, the linear terms in the fluctuations vanish such that $\phi_\alpha(\mathbf{r})$ really minimizes the action [88]. Therefore results in the mean-field approximation could be obtained by minimizing the mean-field grand potential

Ω_0 with respect to ϕ, in analogy to what was presented in the previous chapters. Now, by expanding the action up to Gaussian order in $\eta_\alpha(\mathbf{r},\tau)$ and $\eta^*_\alpha(\mathbf{r},\tau)$, we arrive at the split grand potential $\Omega = \Omega_0 + \Omega_{\mathrm{GF}}$. Where Ω_0 is the mean-field grand potential, while Ω_{GF} takes into account both zero- and finite-temperature fluctuations to the grand-potential.

3.3 Zero-temperature results

3.3.1 Mean-field approximation to the grand-potential

From the analysis of the mean-field contribution to the grand-potential we get the following

$$\frac{\Omega_0}{V} = \sum_{\alpha=1,2} \Big\{ -\mu_\alpha \phi_\alpha^2 + \frac{1}{2} \sum_{\sigma=1,2} \left[g_{\alpha\sigma} + g^{dd}_{\alpha\sigma} \tilde{U}^{dd}(k=0) \right] \phi_\alpha^2 \phi_\sigma^2 \Big\}, \tag{3.4}$$

where

$$\tilde{U}^{dd}(k) = 3\cos^2\theta_k - 1, \tag{3.5}$$

is the Fourier transform of the dipole-dipole interaction [40], (see appendix E for a brief deduction), and θ_k represents the angle between the dipole moment and the momentum k. Now minimizing Ω_0 with respect to ϕ_α, such that $\partial\Omega_0/\partial\phi_\alpha = 0$, we obtain

$$\mu_\alpha = [g_{\alpha\alpha} + \tilde{V}^{dd}_{\alpha\alpha}(k=0)]\phi_\alpha^2 + [g_{\alpha\sigma} + \tilde{V}^{dd}_{\alpha\sigma}(k=0)]\phi_\sigma^2 \tag{3.6}$$

with $\tilde{V}^{dd}_{\alpha\sigma}(k) = g^{dd}_{\alpha\sigma}\tilde{U}(k)$, $\alpha,\sigma = 1,2$ and $\alpha \neq \sigma$. Solving for ϕ_α^2 in Eq. (3.6) we obtain

$$\phi_\alpha^2 = \frac{(g_{\sigma\sigma} + \tilde{V}^{dd}_{\sigma\sigma})\mu_\alpha - (g_{\alpha\sigma} + \tilde{V}^{dd}_{\alpha\sigma})\mu_\sigma}{(g_{\alpha\alpha} + \tilde{V}^{dd}_{\alpha\alpha})(g_{\sigma\sigma} + \tilde{V}^{dd}_{\sigma\sigma}) - [g_{\alpha\sigma} + \tilde{V}^{dd}_{\alpha\sigma}]^2} \tag{3.7}$$

Using Eq. (3.7) into Eq. (3.4) we obtain the grand-canonical potential in the mean-field approximation similar to the Eq. (1.9), with $g^{(0)} \to g + \tilde{V}^{dd}$. From this new grand-potential we can obtain the energy density in the mean-field approximation, which is given by

$$\frac{E_0}{V} = \frac{1}{2} \sum_{\alpha,\sigma=1,2} \left[g_{\alpha\sigma} n_\alpha(\mathbf{r}) n_\sigma(\mathbf{r}) + g^{dd}_{\alpha\sigma} n_\alpha(\mathbf{r}) \int d^3r' U_{dd}(\mathbf{r}-\mathbf{r}') n_\sigma(\mathbf{r}') \right], \tag{3.8}$$

3.3.2 Gaussian fluctuations to the grand-potential

The grand-potential of the Gaussian fluctuations Ω_{GF}, is provided by Eq. (1.10), with the bosonic Matsubara's frequencies $\omega_n = 2\pi n/(\hbar\beta)$, and the 4×4 inverse fluctuation propagator $\mathbb{G}^{-1}$ given as

$$\mathbb{G}^{-1} = \begin{pmatrix} \mathbf{G}_{11}^{-1} & \mathbf{G}_{12}^{-1} \\ \\ \mathbf{G}_{12}^{-1} & \mathbf{G}_{22}^{-1} \end{pmatrix}, \tag{3.9}$$

with the symmetric 2×2 matrices

$$\mathbf{G}_{11}^{-1} = \begin{pmatrix} -\mathrm{i}\hbar\omega_n + \epsilon_k + h_{11} & h_{11} \\ h_{11} & \mathrm{i}\hbar\omega_n + \epsilon_k + h_{11} \end{pmatrix}, \tag{3.10}$$

with

$$h_{11} = \frac{[g_{11} + \tilde{V}_{11}^{dd}(k)]\{[g_{22} + \tilde{V}_{22}^{dd}(k)]\mu_1 - [g_{12} + \tilde{V}_{12}^{dd}(k)]\mu_2\}}{[g_{11} + \tilde{V}_{11}^{dd}(k)][g_{22} + \tilde{V}_{22}^{dd}(k)] - [g_{12} + \tilde{V}_{12}^{dd}(k)]^2}, \tag{3.11}$$

$\mathbf{G}_{22}^{-1} = \mathbf{G}_{11}^{-1}(1 \leftrightarrow 2)$, and

$$\begin{aligned} \mathbf{G}_{12}^{-1} \;&=\; [g_{12} + \tilde{V}_{12}^{dd}(k)] \\ &\times \left\{ \frac{[g_{22} + \tilde{V}_{22}^{dd}(k)]\mu_1 - [g_{12} + \tilde{V}_{12}^{dd}(k)]\mu_2] \times (1 \leftrightarrow 2)}{\left[[g_{11} + \tilde{V}_{11}^{dd}(k)][g_{22} + \tilde{V}_{22}^{dd}(k)] - [g_{12} + \tilde{V}_{12}^{dd}(k)]^2\right]^2} \right\}^{1/2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \end{aligned} \tag{3.12}$$

By solving the determinant of the inverse propagator we get

$$\Omega_{\mathrm{GF}} = \frac{1}{2\beta} \sum_{\substack{k>0 \\ n=-\infty}}^{+\infty} \ln\left[(\hbar^2\omega_n^2 + E_+^2)(\hbar^2\omega_n^2 + E_-^2)\right], \tag{3.13}$$

with the zero-point energy of collective excitations or Bogoliubov spectra given as

$$E_\pm(k, \mu_1, \mu_2, \theta_k) = [\varepsilon^2(k) + 2f_\pm^2(k, \mu_1, \mu_2, \theta_k)\varepsilon(k)]^{1/2}, \tag{3.14}$$

with the free-particle energy $\varepsilon(k) = \hbar^2 k^2/2m$, and the function $f_\pm(k, \mu_1, \mu_2, \theta_k)$ is defined by

$$f_\pm^2 = \frac{\xi}{2}\left[A + B \pm \sqrt{(A-B)^2 + 4\epsilon AB}\right], \tag{3.15}$$

where

$$A = [g_{11} + \tilde{V}_{11}^{dd}(k)]\{[g_{22} + \tilde{V}_{22}^{dd}(k)]\mu_1 - [g_{12} + \tilde{V}_{12}^{dd}(k)]\mu_2\}, \tag{3.16}$$

$$B = [g_{22} + \tilde{V}_{22}^{dd}(k)]\{[g_{11} + \tilde{V}_{11}^{dd}(k)]\mu_2 - [g_{12} + \tilde{V}_{12}^{dd}(k)]\mu_1\}, \tag{3.17}$$

with

$$\xi = \frac{1}{(1-\epsilon)[g_{11} + \tilde{V}_{11}^{dd}(k)][g_{22} + \tilde{V}_{22}^{dd}(k)]}, \tag{3.18}$$

and

$$\epsilon = \frac{[g_{12} + \tilde{V}_{12}^{dd}(k)]^2}{[g_{11} + \tilde{V}_{11}^{dd}(k)][g_{22} + \tilde{V}_{22}^{dd}(k)]}. \tag{3.19}$$

Using the chemical potential given by Eq. (3.6) the Bogoliubov spectra can be written in a more conventional way

$$E_\pm(k, n_1, n_2) = [\varepsilon^2(k) + 2c_\pm^2(k, n_1, n_2)\varepsilon(k)]^{1/2}, \tag{3.20}$$

with $c_\pm$ defined by

$$\begin{aligned} 2c_\pm^2 &= [g_{11} + \tilde{V}_{11}^{dd}(k)]n_1 + [g_{22} + \tilde{V}_{22}^{dd}(k)]n_2 \\ &\pm \{[[g_{11} + \tilde{V}_{11}^{dd}(k)]n_1 - [g_{22} + \tilde{V}_{22}^{dd}(k)]n_2]^2 \\ &+ 4[g_{12} + \tilde{V}_{12}^{dd}(k)]^2 n_1 n_2\}^{1/2}. \end{aligned} \tag{3.21}$$

Performing the sum over Matsubara's frequencies we obtain the Gaussian contributions given by Eqs. (1.17), and (1.18). For now we focus on the study of the grand-potential at zero temperature. However, we will return to thermal effects up later. So taking into account the continuum limit, we have

$$\frac{\Omega_{\rm GF}}{V} = \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} k^2 (E_+ + E_-), \tag{3.22}$$

Now, we consider spherical coordinates. The integral over φ ($0 \leq \varphi \leq 2\pi$) is trivial. To solve the integral over k ($0 \leq k \leq \infty$), we first use the variable change $x_\pm = \hbar k/(2\sqrt{mf_\pm})$. We obtain $\Omega_{\rm GF}/V \sim \int dx_\pm\, x_\pm^3 \sqrt{1 + x_\pm^2} = {\rm B}(2, -5/2)$. The last equality is obtained using $y_\pm = x_\pm^2$ and the definition of the Euler-beta function, see Eq. (D.4), so

$$\frac{\Omega_{\rm GF}}{V} = \frac{4}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2} \int_0^\pi d\theta_k \sin\theta_k \sum_\pm f_\pm^5. \tag{3.23}$$

The respective energy density is given by

$$\frac{E_{\text{GF}}}{V} = \frac{4}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\int_0^\pi d\theta_k \sin\theta_k \sum_\pm c_\pm^5. \tag{3.24}$$

This result is equivalent to those obtained in Refs. [143, 144]. However, it should be taken into account the variable changes $2c_\pm^2 \to V_\pm(\theta_k)$ in Eq. (3) of [143] and $2c_\pm^2 \to I_{E\pm}$ in Eq. (2) of [144].

3.3.3 Equal coupling constants

Now, in order to obtain closed analytical expressions useful simplifications take place when the intra-species and the dipolar coupling constants are equal, such that, $g_{11} = g_{22} = g$ and, $g_{11}^{dd} = g_{22}^{dd} = g^{dd}$. In addition we take the same density in different species $n_1 = n_2 = n/2$. It is also natural to take the same chemical potential, $\mu_1 = \mu_2 = \mu$. From these simplifications we get the following

$$\begin{aligned}\int_0^\pi d\theta_k \sin\theta_k \sum_\pm c_\pm^5 = \left[\frac{1}{2}(g+g_{12})n\right]^{5/2}\int_0^\pi d\theta_k \sin\theta_k[1+\epsilon_{\text{eff}}^+(3\cos^2\theta_k - 1)]^{5/2} \\ + \left[\frac{1}{2}(g-g_{12})n\right]^{5/2}\int_0^\pi d\theta_k \sin\theta_k[1+\epsilon_{\text{eff}}^-(3\cos^2\theta_k - 1)]^{5/2}\end{aligned} \tag{3.25}$$

where

$$\epsilon_{\text{eff}}^+ = \frac{g^{dd}+g_{12}^{dd}}{g+g_{12}}, \qquad \epsilon_{\text{eff}}^- = \frac{g^{dd}-g_{12}^{dd}}{g-g_{12}} \tag{3.26}$$

Since we have a symmetric dipolar interaction we obtain

$$\epsilon_{\text{eff}}^+ = \frac{2a^{dd}}{a \pm a_{12}}, \qquad \epsilon_{\text{eff}}^- = 0. \tag{3.27}$$

We include the $\pm$ signs taking into account how an usual droplet without dipolar interactions can be obtained. So the integral in the second line of Eq. (3.25) is trivial, and the solution of the integral in the first line can be written as

$$\begin{aligned}\int_0^\pi d\theta_k \sin\theta_k[1+\epsilon_{\text{eff}}^+(3\cos^2\theta_k - 1)]^{5/2} &= \int_{-1}^1 dz\,(1-\epsilon_{\text{eff}}^+ + 3\epsilon_{\text{eff}}^+ z^2)^{5/2} \\ &= 2\mathcal{Q}_5(\epsilon_{\text{eff}}^+),\end{aligned} \tag{3.28}$$

where

$$
\begin{aligned}
\mathcal{Q}_5(x) &= \int_0^1 dz\,(1-x+3xz^2)^{5/2} \\
&= \frac{1}{16\sqrt{3x}}\left\{5(x-1)^3 \ln\left[\frac{\sqrt{3x(1-x)}}{\sqrt{3x(1+2x)}+3x}\right]\right. \\
&+ \left.(11+4x+9x^2)\sqrt{3x(1+2x)}\right\},
\end{aligned}
\tag{3.29}
$$

for $x \in \mathbb{R}$. In order to find a better match of the analytical predictions with the experimental results, the solution of the integral in Eq. (3.28) has been considered including cutoffs [33, 145]. However given the resulting forms, the problem translates into something purely computational. Furthermore, each cutoff choice has its own particularities (restrictions, successes, mathematical or physical justification, among others), and the final results for different cutoffs are not necessarily the same. However, such a improvements to deal with the fluctuations in dipolar BECs could eventually be useful from a numerical point of view, as is the case with Eq. (E.13). In this work we use the closed form given by Eq. (3.29). However, the search for an improved form of the dipolar interaction remains an open issue. The function in Eq. (3.29) is real and well-behaved in the interval $-0.5 \leq x \leq 1$, such that $-45\pi\sqrt{6}/256 \leq \mathcal{Q}_5(x) \leq 3\sqrt{3}/2$, ($-1.3527 \leq \mathcal{Q}_5(x) \leq 2.5980$). However, for $x > 1$ due to the logarithmic term $\ln\sqrt{3x(1-x)}$, the function $\mathcal{Q}_5(x)$ becomes complex. We can see that the real $\mathcal{R}\{\mathcal{Q}_5(x)\}$ and the imaginary $\mathcal{I}\{\mathcal{Q}_5(x)\}$ contributions are monotonic increasing functions respectively given as

$$
\begin{aligned}
\mathcal{R}\{\mathcal{Q}_5(x)\} &= \frac{1}{16\sqrt{3x}}\left\{5(x-1)^3 \ln\left[\frac{\sqrt{3x(x-1)}}{\sqrt{3x(1+2x)}+3x}\right]\right. \\
&+ \left.(11+4x+9x^2)\sqrt{3x(1+2x)}\right\}.
\end{aligned}
\tag{3.30}
$$

and,

$$
\mathcal{I}\{\mathcal{Q}_5(x)\} = \frac{5(x-1)^3}{16\sqrt{3x}}\left(\frac{\pi}{2}+2\pi l\right), \tag{3.31}
$$

for $l \in \mathbb{Z}^+$, hereafter for convenience we choose $l = 0$. As l increases, the imaginary contribution becomes of the order of the real one. From these last two contributions we have that $\mathcal{R}\{\mathcal{Q}_5(x)\} > \mathcal{I}\{\mathcal{Q}_5(x)\}$. For example, $\mathcal{I}\{\mathcal{Q}_5(1 \leq x \leq 1.5)\} \sim 0$, and $2.598 \lesssim \mathcal{R}\{\mathcal{Q}_5(1 \leq x \leq 1.5)\} \lesssim 4.621$. In a similar way, as x

increases, we find that $\mathcal{R}\{\mathcal{Q}_5\} \gg \mathcal{I}\{\mathcal{Q}_5\}$, it is therefore reasonable to consider only the real part of the function for $x > 1$. The above analysis contrasts with those is usually implemented in the study of one-component dipolar bosonic gases with the LHY contribution, where $x = a^{dd}/a$, such that for $0 \leq x \leq 1$ we have real values of $\mathcal{Q}_5(x)$. However, in practice the case $x > 1$ is mainly used, given that the dipolar interaction is dominant. Here $a^{dd} > 0$, and to access negative values of x, one could think of using $a < 0$, which is experimentally feasible. However, since the dipolar-LHY term is proportional to $\sim a^{5/2}$, the option in considering an attractive scattering length should be discarded. Regarding $x > 1$ it is also usual to see in literature $\mathcal{Q}_5 = 1 + 3x^2/2$, but this approximation is only valid for $x \to 0$. However, it is used interchangeably for $x > 1$. We consider that a more appropriate mathematical approximation for values greater than 1 but close, could be $\mathcal{Q}_5(x \to 1) = 3\sqrt{3}(3 + 5x^2)/16 + \mathcal{O}((x-1)^3)$. Indeed, taking into account the fluctuations themselves are small and sensitive compared to the leading order provided by the contributions in the mean-field approximation, would be much more appropriate consider the exact solution given by Eq. (3.30) for $x > 1$.

Therefore the energy density for a dipolar Bose-Bose gas including the Gaussian fluctuations becomes

$$\begin{aligned} \frac{E}{V} &= \frac{1}{4}(g+g_{12})n^2(\mathbf{r}) + \frac{1}{2}g^{dd}n(\mathbf{r})\int d^3r' U_{dd}(\mathbf{r}-\mathbf{r}')n(\mathbf{r}') \\ &+ \frac{\sqrt{2}}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\left[(g+g_{12})^{5/2}\mathcal{Q}_5(\epsilon^+_{\text{eff}}) + (g-g_{12})^{5/2}\right]n^{5/2}(\mathbf{r}). \end{aligned} \tag{3.32}$$

The first line represents the energy density in the mean-field approximation, and in the second we have the Gaussian energy density (or the dipolar-LHY energy density). Applying a local-density approximation [33], and using the chemical potential $\mu = \partial E/\partial N$, we obtain the following improved $3d$ GPE including the Gaussian contribution

$$\begin{aligned} i\hbar\frac{\partial\phi(\mathbf{r},t)}{\partial t} &= \Big\{-\frac{\hbar^2}{2m}\nabla^2 + \frac{2\pi\hbar^2}{m}(a+a_{12})|\phi(\mathbf{r},t)|^2 \\ &+ \frac{4\pi\hbar^2}{m}a^{dd}\int d^3r' U_{dd}(\mathbf{r}-\mathbf{r}')|\phi(\mathbf{r}',t)|^2 \\ &+ \frac{16\sqrt{2\pi}}{3}\frac{\hbar^2}{m}\big[(a+a_{12})^{5/2}\mathcal{Q}_5(\epsilon^+_{\text{eff}}) \\ &+ (a-a_{12})^{5/2}\big]|\phi(\mathbf{r},t)|^3\Big\}\phi(\mathbf{r},t). \end{aligned} \tag{3.33}$$

We can see that if a_{12}, and a are repulsive satisfying $a_{12} < a$, the dipolar-LHY term provides a repulsive contribution. This repulsion together with that coming from the mean-field approximation allow stabilize the attraction exerted by the mean-field dipole interaction forming thus a miscible dipolar Bose-Bose droplet. This name is considered since the condition $a_{12} < a$ establishes the miscible region in a self-bound Bose-Bose condensate. However, the formation of stable free immiscible dipolar bosonic droplets can be also achieved. This is possible in the region where $a_{12} > a$. Here the two components separate while still being self-bound due to the same formation mechanism as in the miscible case, i.e. the attraction-repulsion stabilization [143]. In this region the self-bound state is a clear example of the long-range nature of the dipole-dipole interactions. Of course in the immiscible regime the dipolar-LHY term in Eq. (3.33) becomes complex, but if $a_{12} \gtrsim a$ the real part and the imaginary one satisfy $\mathcal{R}\{\text{dipolar-LHY}\} \gg \mathcal{I}\{\text{dipolar-LHY}\}$, such that $(a + a_{12})^{5/2}\mathcal{Q}_5(\epsilon^+_{\text{eff}}) \gg (a - a_{12})^{5/2}$, given that $\mathcal{Q}_5(\epsilon^+_{\text{eff}}) > 1$ for $\epsilon^+_{\text{eff}} > 0$. In other words, the dissipative term (imaginary term), can be neglected. If $a_{12} = a$ we recover the improved GPE used in the study of one-component dipolar gases [146, 147]. For attractive interspecies ($a_{12} < 0$) and repulsive intraspecies ($a > 0$) such that $|a_{12}| < |a|$, we obtain a decrease in the total repulsion, compared to the repulsive scenario above considered. This would, in principle, allow a greater number of atoms to be accommodated in the droplet formation. Of course, without leaving aside that at the mean-field level, the collapse would be present. For $|a_{12}| > |a|$, such that $-1/2 \leq \epsilon^+_{\text{eff}} \leq 0$, where the short-ranged interaction is still dominant with respect to the dipole effect, the term in the third line of Eq. (3.33) becomes imaginary, but if $|a_{12}| \gtrsim |a|$ this term could be smaller than the term in the fourth line, so we could neglected it. The contact interactions in the mean-field become attractive and we would have an usual Bose-Bose droplet plus a weak and attractive dipolar interaction. Since the dominant contribution is not the dipolar one, this would not experimentally relevant. The mean-field contribution given by the contact interaction becomes attractive and we would have an usual Bose-Bose droplet plus a weak and attractive dipolar interaction. In this case we could have a metastable state. Since the dominant contribution is not the dipolar one, this would not experimentally relevant. For $|a_{12}| > |a|$, such that $\epsilon^+_{\text{eff}} < -1/2$ the term in the third line of Eq. (3.33) becomes complex, and this time the imaginary contribution of this term is much greater than the combination of the real one plus the real term given in the last line of Eq. (3.33). In consequence this system is unstable. This could be understood and expected since in the region $\epsilon^+_{\text{eff}} < -1/2$ the combined attraction of the mean-field terms destabilizes the droplet, even taking into account the repulsive effect of the last term in the Eq. (3.33). In other words, the system collapses. Now we focus on the particular case $-a_{12} = a$ applied only in the sector of the fluctuations. In the leading term given by the mean-field approximation we set $-a_{12} \gtrsim a$. This condition was used in Ref. [47] in the study of Bose-Bose droplets as a good approximation to compare the analytical predictions proposal in [23] with results attained with quantum Monte Carlo methods. We write, for convenience, the chemical potential for the Gaussian fluctuations (dipolar-LHY contribution) in the following,

$$\mu_{\rm GF} = \frac{128\sqrt{\pi}}{3}\frac{\hbar^2}{m}\Big[(a^{dd})^{5/2}\frac{\mathcal{Q}_5(\epsilon_{\rm eff}^{+})}{(\epsilon_{\rm eff}^{+})^{5/2}} + a^{5/2}\Big]n^{3/2}. \tag{3.34}$$

This chemical potential is nothing other than the last two lines in Eq. (3.33). Here, by fixing finite values of the scattering length of the dipole-dipole interactions a^{dd}, we have $\epsilon_{\rm eff}^{+} = 2a_{dd}/(|a| - |a_{12}|) \to \infty$. We found that the dipolar term gives a finite value as $\epsilon_{\rm eff}^{+} \to \infty$, where

$$\lim_{\epsilon_{\rm eff}^{+}\to\infty}\frac{\mathcal{Q}_5(\epsilon_{\rm eff}^{+})}{(\epsilon_{\rm eff}^{+})^{5/2}} = \frac{1}{96}[54\sqrt{2} + 5\sqrt{3}\ln{(5-2\sqrt{6})}] \sim 0.5887, \tag{3.35}$$

with which we have a variation of the improved GPE in Eq. (3.33) as follows

$$\begin{aligned} i\hbar\frac{\partial\phi(\mathbf{r},t)}{\partial t} &= \Big\{-\frac{\hbar^2}{2m}\nabla^2 - \frac{2\pi\hbar^2}{m}|a-a_{12}||\phi(\mathbf{r},t)|^2 \\ &+ \frac{4\pi\hbar^2}{m}a^{dd}\int d^3r' U_{dd}(\mathbf{r}-\mathbf{r}')|\phi(\mathbf{r}',t)|^2 \\ &+ \frac{128\sqrt{\pi a^5}}{3}\frac{\hbar^2}{m}\Big[1 + 0.5887\Big(\frac{a^{dd}}{a}\Big)^{5/2}\Big]|\phi(\mathbf{r},t)|^3\Big\}\phi(\mathbf{r},t). \end{aligned} \tag{3.36}$$

While this improved GPE without Gaussian corrections is attractive, the repulsive fluctuations could, at least in principle, stabilize the system a allowing the arise emergence of a new type of droplet. For instance, for atoms of Dy where $a^{dd} = 130.8a_0$ and if $a = 100a_0$ the factor in square brackets is ~ 2.152, which indicates a little more than twice the repulsion in the fluctuations than in a conventional Bose-Bose droplet, although this factor is 0.589 the value of the repulsion in the fluctuations in a conventional one-component dipolar bosonic droplet.

Variational approximation to the miscible droplet

A variational Gaussian ansatz can be used for describing the miscible droplet. Thus for a condensate wave-function given by [40, 143, 144]

$$\phi(\rho, z) = \left(\frac{N}{\pi^{3/2} w_\rho^2 w_z}\right)^{1/2} \exp\left[-\frac{1}{2}\left(\frac{\rho^2}{w_\rho^2} + \frac{z^2}{w_z^2}\right)\right], \tag{3.37}$$

where N is the number of atoms, w_ρ and w_z are the variational widths along the radial ρ and axial z directions, respectively. We substitute this wave-function in the energy

$$\begin{aligned} E &= \int d\mathbf{r} \Big\{ \frac{\hbar^2}{2m} |\nabla\phi(\mathbf{r})|^2 + \frac{\pi\hbar^2}{m}(a + a_{12})|\phi(\mathbf{r})|^4 \\ &+ \frac{2\pi\hbar^2}{m} a^{dd} |\phi(\mathbf{r})|^2 \int d^3r' U_{dd}(\mathbf{r} - \mathbf{r}')|\phi(\mathbf{r}')|^2 \\ &+ \frac{32\sqrt{2\pi}}{15}\frac{\hbar^2}{m}\Big[(a + a_{12})^{5/2} \mathcal{Q}_5(\epsilon_{\text{eff}}^+) + (a - a_{12})^{5/2}\Big] |\phi(\mathbf{r})|^5 \Big\}. \end{aligned} \tag{3.38}$$

This leads to the dipolar energy of miscible droplets

$$\begin{aligned} \frac{E}{N} &= \frac{\hbar^2}{4m}\left(\frac{2}{w_\rho^2} + \frac{1}{w_z^2}\right) + \frac{1}{2\sqrt{2\pi}} \frac{\hbar^2 N}{m w_\rho^2 w_z} [(a + a_{12}) - a_{dd} f(\kappa)] \\ &+ \frac{128}{75\sqrt{5}\pi^{7/4}} \frac{\hbar^2 N^{3/2}}{m w_\rho^3 w_z^{3/2}} \Big[(a + a_{12})^{5/2} \mathcal{Q}_5(\epsilon_{\text{eff}}^+) + (a - a_{12})^{5/2}\Big]. \end{aligned} \tag{3.39}$$

To obtain the dipole-dipole term in the first line we do the following analysis. From the second line in Eq. (3.38), applying the Parseval's theorem and the convolution theorem we obtain [148]

$$E^{dd} = \frac{2\pi\hbar^2}{m} a^{dd} \int \frac{d\mathbf{k}}{(2\pi)^3} \tilde{n}^2(\mathbf{k}) \tilde{U}_{dd}(\mathbf{k}), \tag{3.40}$$

with the Fourier transforms of the density and the dipolar interaction as $\tilde{n}(\mathbf{k}) = \exp[-(k_\rho^2 w_\rho^2 + k_z^2 w_z^2)/4]$ and $\tilde{U}(k) = 3\cos^2\theta_k - 1$ respectively. Now, with the substitution $q = k w_\rho$ and the definition $\kappa = w_\rho / w_z$, considering spherical coordinates, and solving the integrals over the azimuthal angle φ, and the radial distance q, the dipolar energy takes the form

$$\begin{aligned} E^{dd} &= \frac{a^{dd}N^2}{2\sqrt{2\pi}w_\rho^3}\frac{\hbar^2}{m}\int_0^\pi d\theta\,\frac{\sin\theta_k(3\cos\theta_k-1)}{(\sin^2\theta_k+\kappa^{-2}\cos^2\theta_k)^{3/2}} \\ &= -\frac{a^{dd}N^2}{2\sqrt{2\pi}w_\rho^2 w_z}\frac{\hbar^2}{m}f(\kappa). \end{aligned} \tag{3.41}$$

Under the condition $0 \le \kappa < 1$ we have [40, 149, 150], (the $\kappa \ge 1$ case is discussed further below)

$$\begin{aligned} f(\kappa) &= \frac{1}{\kappa}\int_0^1 du\,\frac{1-3u^2}{[1+(\kappa^{-2}-1)u^2]^{3/2}} \\ &= \frac{1}{\kappa}\left[\kappa-\frac{3\kappa^3}{(1-\kappa^2)^{3/2}}\left[\sinh^{-1}\sqrt{\kappa^{-2}-1}-\tanh\left(\sinh^{-1}\sqrt{\kappa^{-2}-1}\right)\right]\right] \\ &= \frac{1+2\kappa^2-3\kappa^2 d(\kappa)}{1-\kappa^2}. \end{aligned} \tag{3.42}$$

In the last line we use the identity $\sinh^{-1}\sqrt{\kappa^{-2}-1} = \tanh^{-1}\sqrt{1-\kappa^2}$, and the function $d\,(\kappa)$ is defined as

$$d(\kappa) = \frac{\tanh^{-1}\sqrt{1-\kappa^2}}{\sqrt{1-\kappa^2}}. \tag{3.43}$$

On the other hand when $\kappa \ge 1$ it is necessary to use the change

$$\frac{\tanh^{-1}\sqrt{1-\kappa^2}}{\sqrt{1-\kappa^2}} \qquad \rightarrow \qquad \frac{\tan^{-1}\sqrt{\kappa^2-1}}{\sqrt{\kappa^2-1}}. \tag{3.44}$$

The function $f(\kappa)$, is monotonically decreasing, and it has asymptotic values for $f\,(\kappa \to \infty) = -2$ (disk-shaped), and $f\,(\kappa \to 0) = 1$ (cigar-shaped). $f(\kappa)$, also changes the sign for $\kappa = 1$, and here $w_\rho = w_z$, so the density distribution of the condensate is spherical and the dipole-dipole interaction has not a contribution.

3.4 Finite-temperature results

We obtain the grand-canonical potential for the equal coupling constants scenario. The thermal Gaussian fluctuations are studied by means of Eq. (1.18)

$$\Omega_{\mathrm{GF}}^{(T)} = \frac{1}{\beta}\sum_{k,\pm}\ln\left(1-e^{-\beta E_\pm(k)}\right), \tag{3.45}$$

in the continuum limit and using spherical coordinates we get

$$\Omega_{\mathrm{GF}}^{(T)} = \frac{1}{(2\pi)^2}\frac{V}{\beta}\sum_{\pm}\int d\theta_k\, dk\, \sin\theta_{k_\pm} k_\pm^2 \ln\left(1 - e^{-\beta E_\pm(k)}\right). \tag{3.46}$$

The momenta $k_\pm$ are obtained from the zero-point energy of collective excitations in Eq. (3.14), where k_+ (k_-) is related to E_+ (E_-). Using

$$\frac{d}{dk}[k^3 \ln(1 - e^{-\beta E})] = 3k^2 \ln(1 - e^{-\beta E}) + \frac{\beta k^3 e^{-\beta E}}{1 - e^{-\beta E}}\frac{dE}{dk}, \tag{3.47}$$

and integrating this relation for $0 \leq k_\pm < \infty$ and assuming the boundary term goes to zero, the Eq. (3.45) becomes

$$\Omega_{\mathrm{GF}}^{(T)} = -\frac{V}{12\pi^2}\sum_{\pm}\int_0^{\pi} d\theta_k \sin\theta_k \int_0^{\infty} dE_\pm \frac{k_\pm^3}{e^{\beta E_\pm} - 1}, \tag{3.48}$$

with

$$k_+ = \left[\frac{2m\mu}{\hbar^2}\left(\sqrt{1 + \frac{x_+^2}{\beta^2\mu^2}} - 1\right)\right]^{1/2}, \tag{3.49}$$

and

$$k_- = \left[\frac{2m\lambda\mu_0}{\hbar^2}\left(\sqrt{1 + \frac{x_-^2}{\beta^2\lambda^2\mu_0^2}} - 1\right)\right]^{1/2}, \tag{3.50}$$

where μ_0 is the chemical potential in absence of the dipole-dipole interactions, λ is given in Eq. (1.23), and we also introduce the variables $x_\pm = \beta E_\pm$. Now, expanding $k_\pm$ at low temperature $k_B T \ll |\mu|$ [44, 45], we get

$$\begin{aligned}
\frac{\Omega_{\mathrm{GF}}^{(T)}}{V} &= -\frac{1}{12\pi^2\beta^4}\left(\frac{m}{\hbar^2\mu_0}\right)^{3/2}\int_0^{\pi} d\theta_k \sin\theta_k [1 + \epsilon_{\mathrm{eff}}^{+}(3\cos^2\theta_k - 1)]^{-3/2} \\
&\times \left[\int_0^{\infty} dx \frac{x^3}{e^x - 1} - \frac{3}{8\beta^2\mu_0^2}[1 + \epsilon_{\mathrm{eff}}^{+}(3\cos^2\theta_k - 1)]^{-2}\int_0^{\infty} dx \frac{x^5}{e^x - 1}\right] \\
&- \frac{1}{6\pi^2\beta^4}\left(\frac{m}{\hbar^2\lambda\mu_0}\right)^{3/2}\left[\int_0^{\infty} dx \frac{x^3}{e^x - 1} - \frac{3}{8\beta^2\lambda^2\mu_0^2}\int_0^{\infty} dx \frac{x^5}{e^x - 1}\right] + \cdots
\end{aligned} \tag{3.51}$$

integrals over x are solved in terms of the Euler's gamma function $\Gamma(x)$, and the Riemann's zeta function $\zeta(x)$ [101] using,

$$\int_0^\infty dx \frac{x^{n-1}}{e^x - 1} = \Gamma(n)\zeta(n), \tag{3.52}$$

and we also found

$$\mathcal{Q}_{-3}(x) = \int_0^1 dz\,(1 - x + 3xz^2)^{-3/2} = \frac{1}{(1-x)\sqrt{1+2x}}, \tag{3.53}$$

and

$$\mathcal{Q}_{-7}(x) = \int_0^1 dz\,(1 - x + 3xz^2)^{-7/2} = \frac{5 + 10x + 9x^2}{5(1-x)^3(1+2x)^{5/2}}. \tag{3.54}$$

These two last functions are real for $-1/2 < x < 1$, and $1 < x < \infty$. In this way the grand-canonical potential becomes

$$\begin{aligned} \frac{\Omega_{\rm GF}^{(T)}}{V} &= -\frac{\pi^2}{90}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{(k_B T)^4}{\mu_0^{3/2}}\left[\mathcal{Q}_{-3}(\epsilon_{\rm eff}^{+}) - \frac{5\pi^2}{7}\mathcal{Q}_{-7}(\epsilon_{\rm eff}^{+})\left(\frac{k_B T}{\mu_0}\right)^2\right] \\ &- \frac{\pi^2}{90}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{(k_B T)^4}{\lambda^{3/2}\mu_0^{3/2}}\left[1 - \frac{5\pi^2}{7}\left(\frac{k_B T}{\lambda\mu_0}\right)^2\right]. \end{aligned} \tag{3.55}$$

Taking into account the leading order at finite-temperature on the grand-potential, we obtain the chemical potential at finite-temperature as

$$\mu_{\rm GF}^{(T)} = -\frac{\sqrt{2\pi}}{240}\left(\frac{m}{\hbar^2}\right)^3\left[\frac{\mathcal{Q}_{-3}(\epsilon_{\rm eff}^{+})}{(a+a_{12})^{3/2}} + \frac{1}{(a-a_{12})^{3/2}}\right]\frac{(k_B T)^4}{n^{5/2}} + \mathcal{O}((k_B T)^6). \tag{3.56}$$

In the miscible regime ($a_{12} < a$), the chemical potential is real, and the miscible droplet is stable. However, in the immiscible ($a_{12} > a$) regime the chemical potential becomes complex, and the imaginary contribution that appears is leading. As a consequence the immiscible droplet undergoes a thermal instability. This is remarkable in comparison to the zero-temperature results. We also can see as providing $a_{12} = a$ in Eq. (3.56) we obtain a thermal instability. However for $-a_{12} = a$, and using $\lim_{\epsilon_{\rm eff}^{+}\to\infty}(\epsilon_{\rm eff}^{+})^{3/2}\mathcal{Q}_{-3}(\epsilon_{\rm eff}^{+}) = -1/\sqrt{2}$, we found the simplified chemical potential at low temperature given by

$$\mu_{\rm GF}^{(T)} = -\frac{\sqrt{\pi}}{480}\left(\frac{m}{\hbar^2}\right)^3\left[1 - \frac{1}{\sqrt{2}}\left(\frac{a}{a^{dd}}\right)^{3/2}\right]\frac{(k_B T)^4}{a^{3/2}n^{5/2}}. \tag{3.57}$$

This finite chemical potential can be found due to the presence of dipole-dipole interactions for binary BECs, contrasting with non-dipolar Bose-Bose mixtures, where the chemical potential at finite-temperature is divergent for $a_{12} = \pm a$.

3.5 Summary and outlook

By considering an effective quantum field theory and using the path integral formalism at Gaussian level (one-loop), we derive the equation of state at zero and low temperature for three-dimensional ultracold Bose-Bose mixtures of atoms with dipole-dipole interactions. In a symmetric scenario, we include an improved GPE on which we focus our analysis regarding the study of some regimes in which the mixture manifests the existence and formation of self-bound droplets. Taking into account that the interspecies interactions act as an additional scale in this problem, these can be used as an extra tool to tune the properties of mixture, so the formation conditions are established mainly by analyzing the relation between the intraspecies and the interspecies scattering lengths. Motivated also by the recent experimental developments in the study of dipolar gases where the relevance of temperature as a control parameter has been considered, we have included some results at low temperature. Contrasting with the finite-temperature non-dipolar Bose-Bose mixtures which are thermally unstable when the attractive interspecies and the repulsive intraspecies are equal, such a instability is not present when the dipole-dipole are included and a stable droplet formation can be achieved.

Although the theory presented in this chapter is initially proposed for atomic systems, in light of recent experimental and theoretical advances at molecular level, it could, at least in principle, be extended to the study of molecular BECs and molecular bosonic droplets. Due to the remarkable progress in the droplets and supersolids research, a clear extension of this chapter is related to the numerical implementation of the proposed GPEs, both at zero and finite temperature. These Eqs. could be suitable for fitting with experimental or numerical evidence. We also consider that these Eqs. could be used in the study of vortex states, and given the experimental relevance of trapping potentials it would be also interesting to consider harmonically trapped mixtures. Due to the finite-temperature results are general for a symmetric dipolar Bose-Bose gas, it could be interesting see how behaves the miscibility-immiscible condition regarding zero-temperature results.

Conclusions

As we can see, each chapter has its own summary and perspectives. Here we include a brief overview highlighting the most relevant features of the work. In this work we have investigated the effects of the fluctuations at Gaussian level (one-loop) of interacting Bose-Bose gases. We focus the analysis on finding regimes where the formation of stable droplets is possible. The main calculations were carried out within an effective field theory by using the path-integral formalism, including some elements of the renormalization by counterterms, and regularization methods. In chapter 1 we consider droplets with nonuniversal corrections to the interactions in three, two, and one dimension, both at zero- and finite-temperature. At zero-temperature we found the following: in three dimensions when we consider the nonuniversal contributions to the interactions as fitting parameters we found a good agreement of our model with some Monte-Carlo results. In two dimensions we only have found small deviations from the equilibrium density regarding usual droplets. In one dimension we obtain a qualitatively agreement with the trend of Monte Carlo results for conventional droplets. Regarding droplets at low temperatures, the difference between intra- and inter-species coupling constants drives the system to a thermal instability in three and two dimensions, but it is not relevant on the formation of one-dimensional droplets. In chapter 2 we research three-dimensional zero-temperature Rabi-coupled Bose-Bose mixtures with nonuniversal corrections to the interactions. Including phase diagrams by tuning the ratio between the inter-species scattering length and the intra-species scattering lengths or the nonuniversal contribution to the interactions, we establish conditions under which the formation and stability of self-bound Rabi-coupled droplets with nonuniversal corrections to the interactions is favorable. Throughout the work we also propose some improved GPEs which could be suitable for fitting with experimental or numerical evidence in the context of free or trapped droplets, and vertex or solitonic states. In chapter 3, and following the path developed in the previous chapters, we adapt the formalism in exploring droplets, both at zero and finite temperature, of Bose-Bose gases with dipole-dipole interactions. We introduce an improved dipolar GPE in which we analyze some conditions under which the stable formation of self-bound miscible or immiscible droplets is possible. We also suggest the possibility of a different kind of dipolar droplet when the attractive interspecies and the repulsive intraspecies are equal. In this droplet the mean-field energy is totally attractive, and it is no present in usual one-component dipolar droplets.

Taking into account the above, a possible extension of this work consists of carrying out a numerical implementation of the suggested models. For instance, it could be interesting to solve the GPEs proposed, or study the validity of our results by means of quantum Monte Carlo techniques. It would be also interesting to extend some of the present results to lower dimensions, including dimensional crossovers. From a more theoretical perspective as an extension of this work we propose the research of the next-leading contributions to the equation of state of Bose-Bose gases and eventually study their possible effects on the droplet formation. In the language of QFT this issue is related to the study of the two-loop corrections to the theory. For our knowledge two loops at zero temperature in Bose-Bose gases remains as an unexplored subject. However, this problem was studied in an one-component Bose gas in the late 1950s [151, 152, 153]. For more recent Refs. we have [154, 155, 156].

The recent years have been very productive in terms of experimental breakthroughs in the study of ultracold gases. These systems have proven to be an versatile platform offering unprecedented controllability in the lab. In particular, two of the most representative experimental groups in the research of atomic dipolar BECs, Pfau's group at the Stuttgart University, and the Ferlaino's group at the Innsbruck University, have carried out a series of experiments, including among others, doplets and supersolidity in a wide range of configurations. Furthermore, the research in ultracold molecule is rapidly expanding, due to key characteristic of obtaining high values of the dipolar strength. All this has given rise to important issues for the future experimental and theoretical research. The understanding of these results in terms of the underlying physics of the Bose-Einstein condensation is a task that is just beginning. For instance, motivated by these experiments, and in order to gain insights, the search of an improved analytical form of the dipolar interaction remains as an open issue. Thermal effects research also deserves an extension in its own right, since these would enable a most controlled handling of the physical properties in quantum matter.

Appendix A

Path integral in quantum mechanics

A.1 Path integral in phase space

It is well know that in a functional integral the functions are the variables of integration. However if the variables are paths, the functional integral is called a path integral. In this appendix we consider some basic aspects related to the path-integral formalism from some sections in Refs. [157, 158] . For simplicity we consider $\hbar = m = 1$. Given a position q at time t, the amplitude for the probability of finding the particle at point q' and time t' is:

$$M(q',t';q,t) = {}_H\langle q',t'|q,t\rangle_H, \tag{A.1}$$

where $|q,t\rangle_H$ is the state, eigenstate of $\hat{q}(t)$ at time t, in the Heisenberg picture. In the Heisenberg picture, operators depend on time, and the state is independent of time. In turn, the operator in the Heisenberg picture $\hat{q}_H(t)$ is related to that in the Schrödinger picture $\hat{q}_S$ by $\hat{q}_H(t) = e^{i\hat{H}t}\hat{q}_S e^{-i\hat{H}t}$, and the Schrödinger picture state is related to the Heisenberg picture state by $|q\rangle = e^{-i\hat{H}t}|q,t\rangle_H$ (t is just a label), and is an eigenstate of $\hat{q}_S$, that is $\hat{q}_S|q\rangle = q|q\rangle$. In terms of the Schrödinger picture, the probability amplitude is given by

$$M(q',t';q,t) = \langle q'|e^{-i\hat{H}(t'-t)}|q\rangle. \tag{A.2}$$

From now on we will drop the index H and S for states, if we write $|q\rangle$ we are in the Schrödinger picture and if we write $|q,t\rangle$ we are in the Heisenberg picture.

In the next lines we derive path-integral representation. We divide the time interval between t and t' into a large number $n+1$ of equal intervals, and we define

$$\epsilon \equiv \frac{t'-t}{n+1}; \qquad t_0 = t, \quad t_1 = t+\epsilon \quad t_{n+1} = t'. \tag{A.3}$$

At any fixed t_i, we have the completeness relation

$$\int dq_i |q_i, t_i\rangle\langle q_i, t_i| = 1. \tag{A.4}$$

If we introduce this relation n times, one for each t_i ($i = 1, ..., n$), in the amplitude, Eq. (A.1), the discrete positions $q_i \equiv q(t_i)$ lead us to obtain a regularized quantum path between q, and q'. This is quantum since at any of the times t_i , the position q can be anything ($q_i \in R$), independent of q_{i-1} , and independent of how small ϵ is. So integrating over all $q_i = q(t_i)$ we integrate over these quantum paths. Denoting $\mathcal{D}q(t) \equiv \prod_{i=1}^{n} dq(t_i)$ we have a *path integral*.

Now, considering that

$$|q\rangle = \int \frac{dp}{2\pi}|p\rangle\langle p|q\rangle, \qquad |p\rangle = \int dq|q\rangle\langle q|p\rangle, \tag{A.5}$$

we have

$$\begin{aligned} {}_H\langle q(t_i), t_i | q(t_{i-1}), t_{i-1}\rangle_H &= \langle q(t_i)|e^{-i\epsilon\hat{H}}|q(t_{i-1})\rangle \\ &= \int \frac{dp(t_i)}{2\pi}\langle q(t_i)|p(t_i)\rangle\langle p(t_i)|e^{-i\epsilon\hat{H}}|q(t_{i-1})\rangle. \end{aligned} \tag{A.6}$$

Requiring the quantum Hamiltonian to be ordered such that all the $\hat{p}$'s are to the left of the $\hat{q}$'s. Then, since we have $\epsilon \to 0$, to first order in ϵ, we get

$$\begin{aligned} M(q', t'; q, t) &= \int \prod_{i=1}^{n} \frac{dp(t_i)}{2\pi} \prod_{j=1}^{n} dq(t_j)\langle q(t_{n+1})|p(t_{n+1})\rangle\langle p(t_{n+1})|e^{-i\epsilon\hat{H}}|q(t_n)\rangle \\ \cdots &\quad \langle q(t_1)|p(t_1)\rangle\langle p(t_1)|e^{-i\epsilon\hat{H}}|q(t_0)\rangle \\ &= \mathcal{D}p(t)\mathcal{D}q(t) \exp\{i[p(t_{n+1})(q(t_{n+1}) - q(t_n)) + \\ \cdots &\quad +p(t_1)(q(t_1) - q(t_0)) - \epsilon(H(p(t_{n+1}), q(t_n)) + \\ \cdots &\quad +H(p(t_1), q(t_0)))]\} \\ &= \mathcal{D}p(t)\mathcal{D}q(t) \exp\left\{i\int_{t_0}^{t_{n+1}} dt[p(t)\dot{q}(t) - H(p(t), q(t))]\right\}, \end{aligned} \tag{A.7}$$

where we have used $q(t_{i+1}) - q(t_i) \to dt\dot{q}(t_i)$. The Eq. (A.7) is called *the path integral in phase space*.

A.2 Path integral in configuration space

To obtain a path integral in configuration space we need the Hamiltonian to be quadratic in momenta ($H(q,p) = p^2/2 + V(q)$), which allows us to use Gaussian integration. If the Hamiltonian is not quadratic in momenta, we have to start in phase space and see what we get in configuration space. The Gaussian integration is over $\mathcal{D}p(t)$, which is

$$\int \mathcal{D}p(\tau) \exp\left\{i \int_t^{t'} d\tau \Big[p(\tau)\dot{q}(\tau) - \frac{1}{2}p^2(\tau)\Big]\right\}. \tag{A.8}$$

In the discrete way this becomes

$$\prod_i \frac{dp(\tau_i)}{2\pi} \exp\left\{i\Delta\tau \Big[p(\tau_i)\dot{q}(\tau_i) - \frac{1}{2}p^2(\tau)\Big]\right\}, \tag{A.9}$$

and using the Gaussian integral

$$\int d^n x \exp\Big[-\Big(\frac{1}{2}x^T A x + b^T x\Big)\Big] = (2\pi)^{n/2} (\det A)^{-1/2} \exp\Big(\frac{1}{2}b^T A^{-1} b\Big), \tag{A.10}$$

with $x_i = p(t_i)$, $A_{ij} = i\Delta\tau\delta_{ij}$, $b = -i\Delta\tau\dot{q}(t_i)$, we get

$$\int \mathcal{D}p(\tau) \exp\{i \int_t^{t'} d\tau [p(\tau)\dot{q}(\tau) - \frac{1}{2}p^2(\tau)]\}, = \mathcal{N} \exp\Big[i \int_t^{t'} dt \frac{1}{2}[\dot{q}(t)]^2\Big], \tag{A.11}$$

$\mathcal{N}$ is a normalization constant. Then the probability amplitude in configuration space is given by

$$M(q',t';q,t) = \mathcal{N} \int \mathcal{D}q \exp\left\{i \int_t^{t'} d\tau \Big[\frac{1}{2}[\dot{q}(\tau)]^2 - V(q)\Big]\right\} = \mathcal{N} \int \mathcal{D}q e^{iS[q]}, \tag{A.12}$$

with the action $S[q] = \int_t^{t'} d\tau L(q(\tau), \dot{q}(\tau))$, and $L = \frac{1}{2}[\dot{q}(t)]^2 - V(q)$.

A.3 Correlation functions

In addition to the probability of transition between (q,t) and (q,t'), we can construct other observables such a the correlation functions. The simplest one is the one-point function $\langle q',t'|\hat{q}(t_a)|q,t\rangle$. If we can make t_a coincides with one of the t_i's in the discretization of the time interval and using the completeness relation, besides the usual products, we also have the expectation value $\langle q_{i+1}, t_{i+1}|\hat{q}(t_a)|q_i, t_i\rangle = q(t_a) = \langle q_{i+1}, t_{i+1}|q_i, t_i\rangle$, since $t_a = t_i \rightarrow q(t_a) = q_i$. The calculation involves the same steps presented above, such that

$$\langle q', t'|\hat{q}(t_a)|q, t\rangle = \int \mathcal{D}q e^{iS[q]} q(t_a). \tag{A.13}$$

For the two-point function $\langle q', t'|\hat{q}(t_b)\hat{q}(t_a)|q, t\rangle$, we have $t_a < t_b$, and $t_a > t_b$. In the first case we obtain the contribution $\int \mathcal{D}q e^{iS[q]} q(t_b)q(t_a)$: in a similar way we have the second scenario $t_a > t_b$. Then, the path integral leads to the two-point function where the $q(t)$'s are time ordering, that is

$$\int \mathcal{D}q e^{iS[q]} q(t_a)q(t_b) = \langle q', t'|T\{\hat{q}(t_a)\hat{q}(t_b)\}|q, t\rangle, \tag{A.14}$$

where time ordering is defined by

$$T\{\hat{q}(t_a)\hat{q}(t_b)\} = \hat{q}(t_a)\hat{q}(t_b)\theta(t_a - t_b) - \hat{q}(t_b)\hat{q}(t_a)\theta(t_b - t_a), \tag{A.15}$$

with $\theta(\tau)$ the step function. Therefore, we can extend the above reasoning and obtain the n-point function or correlation function as

$$G_n(t_{a_1}, ..., t_{a_n}) \equiv \langle q', t'|T\{\hat{q}(t_{a_1})...\hat{q}(t_{a_n})\}|q, t\rangle = \int \mathcal{D}q e^{iS[q]} q(t_{a_1})...q(t_{a_n}). \tag{A.16}$$

Now, we can now define a generating functional

$$Z[J] = \sum_{N \geq 0} = \int dt_1 ... \int dt_N \frac{i^N}{N!} G_N(t_1, ..., t_N)J(t_1)...J(t_N). \tag{A.17}$$

From Eq. (A.16), the integrals factorize, and we obtain

$$Z[J] = \int \mathcal{D}q e^{iS[q]} \sum_{N \geq 0} \frac{1}{N!} \Big[\int dt\, iq(t)J(t) \Big]^N. \tag{A.18}$$

So,

$$Z[J] = \int \mathcal{D}q e^{iS[q,J]} = \int \mathcal{D}q e^{iS[q] + i\int dt J(t)q(t)} \tag{A.19}$$

Therefore we find that this $Z[J]$ generates the correlation functions as

$$\frac{\delta^N Z[J]}{i\delta J(t_1)...i\delta J(t_N)}\Bigg|_{J=0} = \int \mathcal{D}q e^{iS[q]} q(t_1)...q(t_N) = G_N(t_1,...,t_N) \qquad \text{(A.20)}$$

A.4 Euclidean formulation of quantum mechanics

Here we consider the Wick rotation to Euclidean time and the connection of this with the partition function in statistical mechanics. In the development presented in the previous sections we require handled Gaussian integrals of e^{iS}. However, these are not well defined, but if we could have somehow e^S instead of e^{iS}, this would solve the problem. This is what happens when we go to Euclidean space. Consider a time-independent Hamiltonian $\hat{H}$, with a complete set of eigenstates $\{|n\rangle\}$, and eigenvalues $E_n > 0$. Then the transition amplitude can be written as

$$\begin{aligned} {}_H\langle q',t'|q,t\rangle_H &= \langle q'|e^{-i\hat{H}(t'-t)}|q\rangle = \sum_n\sum_m \langle q'|n\rangle\langle n|e^{-i\hat{H}(t'-t)}|m\rangle\langle m|q\rangle \\ &= \sum_n \langle q'|n\rangle\langle n|q\rangle e^{-iE_n(t'-t)} \\ &= \sum_n \psi_n(q')\psi_n^*(q)e^{-iE_n(t'-t)} \qquad \text{(A.21)} \end{aligned}$$

Now consider the analytical continuation to Euclidean time, called Wick rotation, $t'-t \to -i\beta$, we obtain

$$\langle q',\beta|q,0\rangle = \sum_n \psi_n(q')\psi_n^*(q)e^{-\beta E_n}. \qquad \text{(A.22)}$$

For the case $q' = q$ and integrating over q, we obtain the statistical mechanics partition function of a system at a temperature T, with $k_B T = 1/\beta$, (with k_B the Boltzmann constant). So,

$$\int dq \langle q,\beta|q,0\rangle = \int dq \sum_n |\psi_n(q)|^2 e^{-\beta E_n} = \mathrm{Tr}\{\, e^{-\beta\hat{H}}\} = Z[\beta]. \qquad \text{(A.23)}$$

This indicates that in the path integral we need to take closed paths of Euclidean time length β, since $q' \equiv q(t_E = \beta) = q(t_E = 0) \equiv q$. Let see this. The Lagrangian in Minkowski space is

$$L(q,\dot{q}) = \frac{1}{2}\Big(\frac{dq}{dt}\Big)^2 - V(q), \qquad \text{(A.24)}$$

and the exponent in the path integral becomes

$$iS[q] = i\int_0^{t_E=\beta}(-i\,dt_E)\Big[\frac{1}{2}\Big(\frac{dq}{d(-it_E)}\Big)^2 - V(q)\Big] \equiv -S_E[q], \tag{A.25}$$

where by definition, the Euclidean action is

$$S_E[q] = \int_0^{\beta} dt_E\Big[\frac{1}{2}\Big(\frac{dq}{dt_E}\Big)^2 - V(q)\Big], \tag{A.26}$$

We finally get,

$$Z = \mathrm{Tr}\{\, e^{-\beta\hat{H}}\} = \int \mathcal{D}q e^{-S_E[q]}\Bigg|_{q(t_E+\beta)=q(t_E)}. \tag{A.27}$$

As a final comment an useful approximation for any path integral is the *saddle point approximation*, which is the Gaussian integral around a classical solution, an extremum of the action

$$S = S_{cl} + \frac{1}{2}\delta q_i\, S_{ij}\,\delta q_j + \mathcal{O}((\delta q)^3), \tag{A.28}$$

where $S_{cl} = S[q_{cl} : \delta S/\delta q(q_{cl}) = 0]$.

A.5 Quantum-mechanical statistical partition function and correlation functions

In statistical mechanics all the relevant information about the system is encoded in the the partition function, so using this formalism we can calculate any quantity of interest. To calculate the correlation functions, we introduce currents $J(\tau)$, such that

$$Z[\beta; J] = \int \mathcal{D}q e^{-S_E[\beta]+\int_0^\beta J_E(\tau)q_E(\tau)d\tau}. \tag{A.29}$$

So then we can obtain the propagator in imaginary (Euclidean) time as

$$\frac{1}{Z(\beta)}\frac{\delta^2 Z[\beta;J]}{\delta J(\tau_1)\delta J(\tau_2)} = \frac{1}{Z(\beta)}\int \mathcal{D}q(\tau)\, q(\tau_1)q(\tau_2)e^{-S_E(\beta)}, \tag{A.30}$$

we have the Euclidean time τ_i. The $Z[\beta, J]$ was obtained by analytical continuation, this is equal to

$$\langle\Omega|T\{\hat{q}(-i\tau_1)\hat{q}(-i\tau_2)\}\Omega|\rangle_\beta = \frac{1}{Z(\beta)}\mathrm{Tr}[e^{-\beta\hat{H}}T\{\hat{q}(-i\tau_1)\hat{q}(-i\tau_2)\}], \qquad \text{(A.31)}$$

where we consider the vacuum of the interacting theory $|\Omega\rangle$. The operators in Heisenberg picture are also Wick rotated as

$$\hat{q}(t) = e^{i\hat{H}t}\hat{q}e^{-i\hat{H}t} \qquad \rightarrow \qquad \hat{q}(-i\tau) = e^{\hat{H}\tau}\hat{q}e^{-\hat{H}\tau} \qquad \text{(A.32)}$$

A.6 Path integrals from quantum mechanics to quantum field theory

Until now we have seen that a better theory is defined in Euclidean space. This is achieved from Minkowski space by means of Wick rotation to Euclidean space. We can also have that choosing periodic paths, $q(t_E + \beta) = q(\beta)$ in Euclidean time, we get the statistical mechanics partition function as a path integral, for $S_E[q] > 0$. The Euclidean action is positive if the Hamiltonian in the Minkowski space was also positive. In particular, if the periodic paths are infinite ($\beta \rightarrow \infty$), we have the vacuum functional (transition between vacuum states). Therefore, in the extension from quantum mechanics to quantum field theory the vacuum functional is the path integral in Euclidean space over periodic paths of infinite period, with a positive definite Euclidean action. To generalize to field theory, as usual we replace $q_i(t) \rightarrow \phi(t, \vec{x})$. The action in Euclidean space becomes

$$S[\phi] = \int_0^{\hbar\beta} d\tau \int_{L^d} d^d r \mathcal{L}[\phi]. \qquad \text{(A.33)}$$

This action is defined in a d-dimensional box of volume L^d with $d = 3, 2, 1$ the space dimensions. In this work we only consider the Euclidean action, so we have omitted the subscript E, and we have restored the necessary physical constants.

Appendix B

Gaussian fluctuations

In this appendix we introduce some basis on the thermodynamics in the context of quantum field theory (see books in quantum field theory, but preferably in those that consider finite temperature effects, for example [88, 90, 158, 159]). Our starting point is the following action, quadratic in the fluctuations η, η^*

$$S_{\mathrm{GF}}[\eta(k,\omega_n),\eta^*(k,\omega_n)] = \frac{\hbar}{2}\sum_{\substack{k\neq 0\\ n=-\infty}}^{\infty} \eta^*(k,\omega_n)\mathbb{G}^{-1}(k,\omega_n)\eta(k,\omega_n). \tag{B.1}$$

with the bosonic Matsubara's frequencies $\omega_n = 2\pi n/(\hbar\beta)$, and $\mathbb{G}^{-1}(k,\omega_n)$ is defined, for instance, in Eq. (1.11). In such a case the partition function (the generating functional) is given by [90]

$$\begin{aligned}
\mathcal{Z}_{\mathrm{GF}} &= \int \mathcal{D}[\eta,\eta^*] \exp\Big[-\frac{1}{2}\sum_{k,\omega_n}\eta^*(k,\omega_n)\mathbb{G}^{-1}(k,\omega_n)\eta(k,\omega_n)\Big] \\
&= \prod_{\substack{k\neq 0\\ \omega_n\neq 0}} [\det \mathbb{G}(k,\omega_n)]^{1/2} = \exp\Big[\frac{1}{2}\sum_{k,\omega_n\neq 0} \ln\det\mathbb{G}(k,\omega_n)\Big].
\end{aligned} \tag{B.2}$$

Formally, in second line of Eq. (B.2) we have a constant $\mathcal{N}$ coming from Gaussian bosonic integration. However, it can be drooped, since it has not effect the thermal properties [90]. Now, we consider $\Omega_{\mathrm{GF}} = -\beta^{-1}\ln\mathcal{Z}_{\mathrm{GF}}$ the grand-canonical potential for the Gaussian fluctuations. So

$$\Omega_{\mathrm{GF}} = -\frac{1}{2\beta}\sum_{k,\omega_n\neq 0}\ln\det\mathbb{G} = \frac{1}{2\beta}\sum_{k,\omega_n\neq 0}\ln[\det(\mathbb{G}^{-1})], \tag{B.3}$$

the last term can be obtained considering that the matrix propagator $\mathbb{G}$ can be inverted, and we use the property $\det(\mathbb{G}\mathbb{G}^{-1}) = \det(I) = 1$, with I the unit matrix.

Solving the determinant of the inverse propagator, we get

$$\begin{aligned}
\Omega_{\text{GF}} &= \frac{1}{2\beta}\sum_{\substack{k>0\\ n=-\infty}}^{+\infty} \ln\left[(\hbar^2\omega_n^2 + E_+^2(k))(\hbar^2\omega_n^2 + E_-^2(k))\right] \\
&= \frac{1}{2\beta}\sum_{\substack{k>0\\ n=-\infty}}^{+\infty} \ln[\hbar^2\omega_n^2 + E_+^2(k)] + \frac{1}{2\beta}\sum_{\substack{k>0\\ n=-\infty}}^{+\infty} \ln[\hbar^2\omega_n^2 + E_-^2(k)] \\
&\equiv \Omega_{\text{GF}}^+ + \Omega_{\text{GF}}^-. \qquad \text{(B.4)}
\end{aligned}$$

To solve the Matsubara sum , we can use the partition function in the Euclidean path integral formalism for a harmonic oscillator [90]. From Eq. (A.29) we have

$$\mathcal{Z}[\beta; J] = \int \mathcal{D}q(\tau) e^{-\int_0^\beta d\tau\left[\frac{m}{2}\left(\frac{dq}{d\tau}\right)^2 + \frac{1}{2}m\omega^2 q^2 - Jq\right]}. \qquad \text{(B.5)}$$

Integrating by parts the kinetic term and applying the periodic conditions of the Euclidean space the boundary contribution is zero and we have

$$\int d\tau\left(\frac{dq}{d\tau}\right)^2 = -\int d\tau q \frac{d^2 q}{d\tau^2}. \qquad \text{(B.6)}$$

So the partition function becomes in a bosonic Gaussian integral given by [90, 160]

$$\begin{aligned}
\mathcal{Z}[\beta; J] &= \int \mathcal{D}q(\tau) e^{-\int_0^\beta d\tau\left[\frac{1}{2}q\left(-m\frac{d^2}{d\tau^2} + m\omega^2\right)q - Jq\right]} \\
&= \mathcal{Z}(\beta) e^{\frac{1}{2}\int d\tau d\tau' J(\tau)K(\tau,\tau')J(\tau')}. \qquad \text{(B.7)}
\end{aligned}$$

In Eq. (B.7) the propagator $K(\tau, \tau')J(\tau')$ is the inverse of $-md^2/d\tau^2 + m\omega^2$, such that

$$\left(-m\frac{d^2}{d\tau^2} + m\omega^2\right)K(\tau, \tau') = \delta(\tau - \tau'), \qquad \text{(B.8)}$$

with the free propagator

$$K(\tau, \tau') = \Delta_{\text{free}}(\tau - \tau'), \qquad \text{(B.9)}$$

which is defined by $\Delta_{\text{free}}(\tau - \tau') \equiv \langle T\{\hat{q}(-i\tau)\hat{q}(-i\tau')\}\rangle$, with the periodic condition $\Delta_{\text{free}}(\tau - \beta) = \Delta_{\text{free}}(\tau)$ for any value of τ in the interval $[0, \beta]$.

Now, for simplicity we consider $m = 1$. The solution of Eq. (B.8) in the interval

$[0, \beta]$, with the mentioned periodic condition can be obtained in the following

$$\begin{aligned} K &= Ae^{\omega\tau} + Be^{-\omega\tau} \qquad \text{for} \qquad \tau < \tau' \\ K &= Ce^{\omega\tau} + De^{-\omega\tau} \qquad \text{for} \qquad \tau > \tau', \end{aligned} \tag{B.10}$$

imposing continuity at $\tau = \tau'$

$$(A - C)e^{\omega\tau'} = (D - B)e^{-\omega\tau'}. \tag{B.11}$$

However, $dK/d\tau$ is not continuous at $\tau = \tau'$, here we get

$$-\int_{\tau'-\epsilon}^{\tau'+\epsilon} d\tau \, \frac{d^2K}{d\tau^2} + \omega^2 \int_{\tau'-\epsilon}^{\tau'+\epsilon} d\tau \, K = \int_{\tau'-\epsilon}^{\tau'+\epsilon} d\tau \, \delta(\tau - \tau'), \tag{B.12}$$

when ϵ goes to zero we have

$$\left.\frac{dK}{d\tau}\right|_{\tau'-\epsilon} - \left.\frac{dK}{d\tau}\right|_{\tau'+\epsilon} = 1, \tag{B.13}$$

so for $\tau = \tau'$ we obtain

$$\omega[(A - C)e^{\omega\tau'} - (B - D)e^{-\omega\tau'}] = 1. \tag{B.14}$$

For Eqs. (B.11) and (B.14) we have

$$A - B = \frac{e^{-\omega\tau'}}{2\omega} \qquad\qquad C - D = -\frac{e^{\omega\tau'}}{2\omega}, \tag{B.15}$$

and using $A - B$ in the first Eq. (B.10) and $C - D$ in the second Eq. (B.10) we obtain

$$K = A_1(e^{\omega\tau} + e^{-\omega\tau}) + \frac{1}{2\omega}e^{-\omega|\tau-\tau'|}. \tag{B.16}$$

Then,

$$\Delta_{\text{free}}(\tau) = A_1(e^{\omega\tau} + e^{-\omega\tau}) + \frac{1}{2\omega}e^{-\omega|\tau|}, \tag{B.17}$$

for $\tau = \beta$ we have $\Delta_{\text{free}}(0) = \Delta_{\text{free}}(\beta)$, and

$$A_1 = \frac{1}{2\omega} \frac{e^{-\beta\omega} - 1}{2 - e^{\beta\omega} - e^{-\beta\omega}}. \tag{B.18}$$

By means of the trigonometric identities $2 - e^{\beta\omega} - e^{-\beta\omega} = 4\sinh^2(\beta\omega/2)$, and $e^{-\beta\omega} - 1 = 2e^{-\beta\omega/2}\sinh^2(\beta\omega/2)$ we have

$$A_1 = \frac{1}{2\omega}\frac{1}{e^{\beta\omega}-1}. \tag{B.19}$$

Therefore,

$$\Delta_{\text{free}}(\tau) = \frac{1}{2\omega}\left[(1+n(\omega))e^{-\omega\tau} + n(\omega)e^{\omega\tau}\right], \tag{B.20}$$

with $n(\omega) = 1/(e^{\beta|\omega|} - 1)$ the Bose-Einstein distribution.

From Eq. (B.7) and using the same procedure as with the bosonic gas, for the harmonic oscillator we obtain

$$\Omega_{\text{HO}} = \frac{1}{2\beta}\sum_{\substack{k>0 \\ n=-\infty}}^{+\infty} \ln\left(\hbar^2\omega_n^2 + \hbar^2\omega^2\right). \tag{B.21}$$

Therefore, in this way we can see that for the Bose-Bose gas we have

$$\Delta_{\pm}(\tau) = \frac{1}{2E_{\pm}}\left[(1+n(E_{\pm}))e^{E_{\pm}\tau} + n(E_{\pm})e^{E_{\pm}\tau}\right], \tag{B.22}$$

with $n(E_{\pm}) = 1/(e^{\beta E_{\pm}} - 1)$.

From Eq. (B.4) we get

$$\begin{aligned} \frac{1}{2E_{\pm}}\frac{d\Omega_{\text{GF}}^{\pm}}{dE_{\pm}} &= \sum_{k,\pm}\Delta(\tau=0) \\ \frac{d\Omega_{\text{GF}}^{\pm}}{dE_{\pm}} &= \frac{1}{2}\sum_{k,\pm}\left(1 + \frac{2}{e^{\beta E_{\pm}}-1}\right), \end{aligned} \tag{B.23}$$

So

$$\begin{aligned} \Omega_{\text{GF}}^{\pm} &= \frac{1}{2}\sum_{k,\pm}\left[\int_0^{E_{\pm}} dE'_{\pm}\left(1+\frac{2}{e^{\beta E'_{\pm}}-1}\right)\right] \\ &= \frac{1}{2}\sum_{k,\pm}\left[E_{\pm}(k) + \frac{2}{\beta}\ln\left(1-e^{-\beta E_{\pm}(k)}\right) + \text{constant}\right], \end{aligned} \tag{B.24}$$

where the constant is divergent, but taking into account that this is independent of temperature and the energies we can neglect it [90]. There are different ways to solve the Matsubara sum [88, 159, 161]. For example, this can be obtained by means of some logarithmic identities, contour integration, and the residue theorem.

Appendix C

The coupling constants

C.1 The two-body problem

This appendix is based mainly on the Ref. [95]. Let us consider the Hamiltonian operator of a particle

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_r} + \hat{V}, \tag{C.1}$$

with momentum $\hat{\mathbf{p}}$ and reduced mass m_r ($m_r = m/2$ two identical particles, each of mass m), while $\hat{V}$ is the interaction potential operator. We consider $|\mathbf{r}\rangle$ as the eigenstate of the position operator $\hat{\mathbf{r}}$, such that $\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle$, and the potential operator $\hat{V}$ diagonal in the coordinate representation, $\hat{V}|\mathbf{r}\rangle = V(\mathbf{r})|\mathbf{r}\rangle$.

As shown in different textbooks [93, 94], in d spatial dimensions, the matrix element $T_{\mathbf{k}\mathbf{k}'} = \langle\mathbf{k}|\hat{T}|\mathbf{k}'\rangle$ of the transition operator $\hat{T}$ of scattering theory satisfies the T-matrix equation

$$T_{\mathbf{k}\mathbf{k}'} = V_{\mathbf{k}\mathbf{k}'} + \int d^d k'' \frac{V_{\mathbf{k}\mathbf{k}''}}{\frac{\hbar^2 k^2}{2m_r} - \frac{\hbar^2 (k'')^2}{2m_r} + i\epsilon} T_{\mathbf{k}''\mathbf{k}'} \tag{C.2}$$

where $|\mathbf{k}\rangle$ is the initial state, $|\mathbf{k}''\rangle$ is an intermediate state, $|\mathbf{k}'\rangle$ is the final state, $V_{\mathbf{k}\mathbf{k}'} = \langle\mathbf{k}|\hat{V}|\mathbf{k}'\rangle$, and $\epsilon > 0$ ensure that in the scattering there are only outgoing waves. Here, $|\mathbf{k}\rangle$, $|\mathbf{k}'\rangle$, and $|\mathbf{k}''\rangle$ are eigenstates of the momentum operator $\hat{\mathbf{p}}$. We also consider the Fourier transform of the interaction potential $V(\mathbf{r})$, as $\tilde{V}(\mathbf{k}) = \int d^D\mathbf{r}\, V(r)\, e^{-i\mathbf{k}\cdot\mathbf{r}}$ such that $V_{\mathbf{k}\mathbf{k}'} = \tilde{V}(\mathbf{k}-\mathbf{k}')/(2\pi)^d$. We assume that the interaction potential is spherically symmetric, i.e. $V(\mathbf{r}) = V(r)$ with $r = |\mathbf{r}|$, so $\tilde{V}(\mathbf{k}) = \tilde{V}(k)$.

C.2 Partial waves decomposition

Defining the partial wave expansion of $V_{\mathbf{kk}'}$, substituting this into Eq. (C.2), using the orthogonality of Legendre functions and the uniqueness of the representation in partial waves, we get

$$\begin{aligned} T_l(k,k')P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}') &= V_l(k,k')P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}') + \int \frac{d^dk''}{(2\pi)^d}\left[\frac{N(d,l)}{\frac{\hbar^2k^2}{m}-\frac{\hbar^2(k'')^2}{m}+i\epsilon}\right. \\ &\times \left. V_l(k,k'')T_l(k'',k')P_l(\hat{\mathbf{k}}''\cdot\hat{\mathbf{k}}')\right] \end{aligned} \tag{C.3}$$

where [162]

$$N(d,l) = \frac{2l+d}{l}\binom{d+l-3}{l-1} = \frac{2l+d}{l}\frac{(d+l-3)!}{(l-1)!(d-2)!}. \tag{C.4}$$

For $k = k'$, using the orthonormalization of Legendre polynomials the angular integral is calculated, and choosing the s-wave term $l = 0$ we obtain

$$\begin{aligned} T_{l=0}(k) &= V_{l=0}(k) \\ &+ \frac{2\pi^{d/2}}{\Gamma(d/2)}\int_0^\infty \frac{dk''}{(2\pi)^d}\frac{(k'')^{d-1}}{\frac{\hbar^2k^2}{m}-\frac{\hbar^2(k'')^2}{m}+i\epsilon}V_{l=0}(k,k'')T_{l=0}(k'',k), \end{aligned} \tag{C.5}$$

where $T_{l=0}(k) = T_{l=0}(k,k)$, $V_{l=0}(k) = V_{l=0}(k,k)$, and $\Gamma(x)$ the Euler-gamma function.

C.3 On-shell approximation

We consider the s-wave approximation and the on-shell approximation [93]. For $k \simeq k''$ we have $T_{l=0}(k'',k) \simeq T_{l=0}(k,k) = T_{l=0}(k)$ and $V_{l=0}(k,k'') \simeq V_{l=0}(k,k) = V_{l=0}(k)$. So Eq. (C.5) becomes

$$T_{l=0}(k) = V_{l=0}(k) + V_{l=0}(k)C(k)T_{l=0}(k) \tag{C.6}$$

such that

$$T_{l=0}(k) = \frac{1}{[V_{l=0}(k)]^{-1}-C(k)}, \tag{C.7}$$

where in the limit $\epsilon \to 0$, and using dimensional regularization, we have

$$\begin{aligned} C(k) &= -\frac{\pi^{d/2}}{\Gamma(d/2)} \int_0^\infty \frac{dk''}{(2\pi)^d} \frac{(k'')^{d-1}}{\frac{\hbar^2 k^2}{m} - \frac{\hbar^2 (k'')^2}{m}} \\ &= -\frac{m}{\hbar^2}(-ik)^{d-2} \frac{\mathrm{B}(d/2, 1-d/2)}{(4\pi)^{d/2}\Gamma(d/2)}. \end{aligned} \tag{C.8}$$

Here we use definition of the Euler-beta function

$$\mathrm{B}(a,b) = \int_0^\infty dt \frac{t^{a-1}}{(1+t)^{a+b}} \qquad \mathcal{R}\{a\}, \mathcal{R}\{b\} > 0 \tag{C.9}$$

and the relation $B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$.

This constant in Ref. [95], Eq. 9, is not complete. However when it is used later the problem has been solved. From usual properties of Gamma function we have for $d = 3$, and $d = 1$, respectively

$$C_{d=3}(k) = -i\frac{m}{4\pi\hbar^2}k \qquad\qquad C_{d=1}(k) = -i\frac{m}{2\hbar^2}\frac{1}{k} \tag{C.10}$$

For $d = 2$ we obtain $\Gamma(0)$, so in this case we use dimensional regularization in the modified minimal subtraction scheme, and we get

$$C_{d=2}(k) = \frac{m}{2\pi\hbar^2} \ln\left(\frac{k}{\sqrt{\epsilon_c}}\right) - \frac{m}{4\hbar^2}\mathrm{i}, \tag{C.11}$$

with the low-energy cutoff $\epsilon_c = \hbar^2\bar{\kappa}^2/m$.

Appendix D

Renormalization by counterterms and regularization methods

D.1 Dimensional regularization

We have the grand-canonical potential given by [51, 82]

$$\frac{\Omega^{\pm}_{\mathrm{GF}}}{L^d} = \frac{1}{2}\frac{S_d}{(2\pi)^d}\int_0^{\infty} dk\, k^{d-1}\sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2c_{\pm}^2\right)}, \tag{D.1}$$

with $S_d = 2\pi^{d/2}/\Gamma(d/2)$ the solid angle in d dimensions and $\Gamma(x)$ the Euler gamma function, and $2c_{\pm} = g_{11}n_1 + g_{22}n_2 \pm \sqrt{(g_{11}n_1 - g_{22}n_2)^2 + 4g_{12}^2 n_1 n_2}$. For convenience $c_{\pm}^2 = f$ in Eq. (1.15), but expressed in terms of the density. In the following we use dimensional regularization. So considering the following substitution $x_{\pm} = \hbar k/\left(2\sqrt{mc_{\pm}^2}\right)$, we have

$$\frac{\Omega^{\pm}_{\mathrm{GF}}}{L^d} = \frac{S_d\, c_{\pm}^2}{(2\pi)^d}\left(\frac{2}{\hbar}\sqrt{mc_{\pm}^2}\right)^d \int_0^{\infty} dx\, x_{\pm}^{d-1} x_{\pm}\sqrt{x_{\pm}^2 + 1}. \tag{D.2}$$

Using $u_{\pm} = x_{\pm}^2$, we have

$$\frac{\Omega^{\pm}_{\mathrm{GF}}}{L^d} = \frac{S_d\, c_{\pm}^2}{2(2\pi)^d}\left(\frac{2}{\hbar}\sqrt{mc_{\pm}^2}\right)^d \int_0^{\infty} du_{\pm}\, u_{\pm}^{\frac{d-1}{2}}(1+u_{\pm})^{\frac{1}{2}}. \tag{D.3}$$

Now, considering the beta-Euler function

$$\mathrm{B}(a,b) = \int_0^{\infty} dt \frac{t^{a-1}}{(1+t)^{a+b}} \qquad \mathcal{R}\{a\}, \mathcal{R}\{b\} > 0, \tag{D.4}$$

expressed in terms of the Gamma function

$$\Gamma(z) = \int_0^{\infty} dt\, t^{z-1} e^{-t} \mathcal{R}\{z\} > 0, \tag{D.5}$$

we obtain

$$\mathrm{B}(a,b)=\frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}. \tag{D.6}$$

Therefore the grand-canonical potential for the Gaussian contributions is

$$\Omega^{(0)}_{\mathrm{GF}}=\frac{L^d}{\Gamma(d/2)}\left(\frac{m}{\pi\hbar}\right)^{d/2}\mathrm{B}\left(\frac{1+d}{2},-\frac{2+d}{2}\right)(c_+^{d+2}+c_-^{d+2}). \tag{D.7}$$

We can obtain closed expressions for $d=3$, and $d=1$, such that:

For $d=3$

$$\frac{\Omega^{(0)}_{\mathrm{GF}}}{L^3}=\frac{8}{15\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\sum_{\pm}c_{\pm}^5. \tag{D.8}$$

For $d=1$

$$\frac{\Omega^{(0)}_{\mathrm{GF}}}{L}=-\frac{2}{3\pi}\left(\frac{m}{\hbar^2}\right)^{1/2}\sum_{\pm}c_{\pm}^3. \tag{D.9}$$

However, for $d=2$ we obtain

$$\frac{\Omega^{(0)}_{\mathrm{GF}}}{L^2}\sim\mathrm{B}\left(\frac{3}{2},-2\right) \tag{D.10}$$

Therefore, the two-dimensional case needs to be considered in a different way.

D.2 Two-dimensional renormalization by counterterms

We consider an one-component Bose gas for simplicity, the Bose-Bose gas can be analyzed in an analogous way. So, taking into account the following Lagrangian, where the subscript zero indicates bare quantities (that means non-physical quantities) [163, 164]. So

$$\mathcal{L}_0=\phi_0^*(\mathbf{r},\tau)\left(\hbar\frac{\partial}{\partial\tau}-\frac{\hbar^2}{2m}\nabla^2-\mu_0\right)\phi_0(\mathbf{r},\tau)+\frac{1}{2}g_0|\phi_0(\mathbf{r},\tau)|^4 \tag{D.11}$$

To solve the divergence of the grand-potential we rewrite the Lagrangian to obtain a physical or renormalized Lagrangian (variables without the subscript zero) plus the counterterms. These counterterms are responsible for canceling the divergence. So defining $\phi_0 = Z^{1/2}\phi$ and $\phi_0^* = Z^{1/2}\phi^*$, with Z the field strength renormalization. Replacing these bare fields into (D.11), and taking $Z \equiv 1 + \delta Z$, $g_0 Z^2 \equiv g\delta Z_g \equiv g(1+\delta g)$, $\mu_0 Z \equiv \mu\delta Z_\mu \equiv \mu(1+\delta\mu)$. These definitions have been chosen to obtain the following Lagrangian

$$\begin{aligned}
\mathcal{L}_0 &\rightarrow \mathcal{L} + \delta Z\phi^*(\mathbf{r},\tau)\Big(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2\Big)\phi(\mathbf{r},\tau) + \frac{1}{2}g\delta g|\phi|^4 - \mu\delta\mu|\phi|^2 \\
&\rightarrow \mathcal{L} + \frac{1}{2}g\delta g|\phi|^4 - \mu\delta\mu|\phi|^2 \\
&= \mathcal{L}(g \rightarrow g(1+\delta g), \mu \rightarrow \mu(1+\delta\mu)). \qquad \text{(D.12)}
\end{aligned}$$

In the second term of first line we choose $\delta Z = 0$ because the term in brackets is physical, and it does not need renormalization. Using the Lagrangian in the third line of Eq. (D.12), we obtain the Gaussian contribution to the grand canonical potential of the two-dimensional Bose gas by

$$\begin{aligned}
\Omega_{\mathrm{GF}} &= \Omega - \Omega_0 \\
&= \Omega + \frac{\mu^2 L^2}{2g} \\
&= \lim_{d\to 2}\bar{\kappa}^{2-d}\frac{2\pi^{d/2}L^d}{\Gamma(d/2)}\frac{(2\mu)^{\frac{d}{2}+1}}{4(2\pi)^d}\left(\frac{2m}{\hbar^2}\right)^{d/2}\frac{\Gamma(\frac{1+d}{2})\Gamma(-\frac{2+d}{2})}{\Gamma(-\frac{1}{2})} \\
&+ \frac{\mu^2L^2}{2g}\delta g - \frac{\mu^2 L^2}{g}\delta\mu. \qquad \text{(D.13)}
\end{aligned}$$

In obtaining the third line we consider dimensional regularization given by Eq. (D.1) for $c_\pm^2 \rightarrow \mu$, and as a result we get an expression similar to Eq. (D.7). However, it should be noted that strictly Eq. (D.1) does not have the correct physical dimensions. Indeed to solve this issue we need to include a dimensional multiplicative factor κ in front of this integral. The specific factor may vary but in general it should be something like $\sim \kappa^{d_i - d}$ for $d_i = 1, 2, 3$. The convenience of one or another factor mainly depends on the intention to simplify some numerical factors, which arise in later stages. In other situations the main idea is to be able to compare the results with the literature. Thus, taking into account these two scenarios we consider

$$dk^2 \rightarrow \bar{\kappa}^{2\bar{\epsilon}}dk^d, \qquad \bar{\kappa} \equiv \frac{e^{\gamma/2}L}{2\sqrt{\pi}}\kappa, \qquad 2\bar{\epsilon} \equiv 2 - d, \qquad \text{(D.14)}$$

with $\gamma \sim 0.5772$ de Euler-Mascheroni constant.

As a result we have

$$\begin{aligned}\frac{\Omega_{\mathrm{GF}}}{L^2} &= -\lim_{\bar{\epsilon}\to 0}\frac{\mu\,\bar{\kappa}^{2\bar{\epsilon}}}{2\sqrt{\pi}}\left(\frac{m\mu L^2}{\pi\hbar^2}\right)^{1-\bar{\epsilon}}\frac{\Gamma(\frac{3}{2}-\bar{\epsilon})\Gamma(-2+\bar{\epsilon})}{\Gamma(1-\bar{\epsilon})}\\ &+ \frac{\mu^2}{2g}\delta g - \frac{\mu^2}{g}\delta\mu. \end{aligned} \tag{D.15}$$

To solve this limit we use the following expansions of the Gamma function [92]

$$\begin{aligned}\Gamma\left(\frac{3}{2}-\bar{\epsilon}\right) &= \Gamma\left(\frac{3}{2}\right)\left[1-\bar{\epsilon}\psi\left(\frac{3}{2}\right)+\frac{1}{2}\bar{\epsilon}^2\left[\psi'\left(\frac{3}{2}\right)+\psi^2\left(\frac{3}{2}\right)\right]\right]+\mathcal{O}(\bar{\epsilon}^3),\\ \Gamma(-2+\bar{\epsilon}) &= \frac{1}{2}\left[\frac{1}{\bar{\epsilon}}+\psi(3)+\frac{1}{2}\bar{\epsilon}\left[\frac{\pi^2}{3}+\psi^2(3)-\psi'(3)\right]\right]+\mathcal{O}(\bar{\epsilon}^2),\\ \Gamma(1-\bar{\epsilon}) &= \Gamma(1)\left[1-\bar{\epsilon}\psi(1)+\frac{1}{2}\bar{\epsilon}^2\left[\psi'(1)+\psi^2(1)\right]\right]+\mathcal{O}(\bar{\epsilon}^3), \end{aligned} \tag{D.16}$$

with the Euler digamma function $\psi(z) = \frac{d}{dz}\ln\Gamma(z)$. So,

$$\frac{\Gamma(\frac{3}{2}-\bar{\epsilon})\Gamma(-2+\bar{\epsilon})}{\Gamma(1-\bar{\epsilon})} = \frac{1}{2}\Gamma\left(\frac{3}{2}\right)\left[\frac{1}{\bar{\epsilon}}+\ln 4-\frac{1}{2}-\gamma\right]+\mathcal{O}(\bar{\epsilon}), \tag{D.17}$$

and expanding the remaining term in Eq. (D.15) we obtain

$$\begin{aligned}\frac{\Omega_{\mathrm{GF}}}{L^2} &= -\lim_{\bar{\epsilon}\to 0}\frac{\mu}{2\sqrt{\pi}}\left(\frac{m\mu L^2}{\pi\hbar^2}\right)\left[1+\bar{\epsilon}\ln\left(\frac{\pi\hbar^2}{m\mu L^2}\right)\right]\left[1+\bar{\epsilon}\ln\left(\frac{e^{\gamma}L^2\kappa^2}{4\pi}\right)\right]\\ &\times \frac{\sqrt{\pi}}{4}\left[\frac{1}{\bar{\epsilon}}+\ln\left(\frac{4}{e^{1/2+\gamma}}\right)\right]+\frac{\mu^2}{2g}\delta g-\frac{\mu^2}{g}\delta\mu \end{aligned} \tag{D.18}$$

So

$$\frac{\Omega_{\mathrm{GF}}}{L^2} = -\frac{m\mu^2}{8\pi\hbar^2}\left[\frac{1}{\bar{\epsilon}}+\ln\left(\frac{\hbar^2\kappa^2}{\sqrt{e}m\mu}\right)\right]+\frac{\mu^2}{2g}\delta g-\frac{\mu^2}{g}\delta\mu \tag{D.19}$$

In order to deal with the divergence of Eq. (D.19) which has been isolated by dimensional renormalization and evidenced by the simple pole of the gamma function, we consider the modified minimal subtraction scheme $\overline{\mathrm{MS}}$-scheme [163, 164]. In the essence of $\overline{\mathrm{MS}}$-scheme the counterterms can be used as appropriate to solve the divergence. Therefore [154, 155] $\delta\mu = 0$, and the only counterterm non-zero is that related to the coupling constant

$$\delta g = \frac{mg}{4\pi\hbar^2}\frac{1}{\bar{\epsilon}}. \tag{D.20}$$

So

$$\frac{\Omega_{\mathrm{GF}}}{L^2} = -\frac{m\mu^2}{8\pi\hbar^2}\ln\left(\frac{\hbar^2\kappa^2}{\sqrt{e}m\mu}\right), \tag{D.21}$$

and

$$\frac{\Omega}{L^2} = -\frac{\mu^2}{2g} - \frac{m\mu^2}{8\pi\hbar^2}\ln\left(\frac{\hbar^2\kappa^2}{\sqrt{e}m\mu}\right). \tag{D.22}$$

From the $2 \to 2$ atomic scattering we know that [165]

$$\frac{1}{g} = \frac{m}{4\pi\hbar^2}\ln\left(\frac{4}{a^2e^{2\gamma}\kappa^2}\right). \tag{D.23}$$

This term precisely cancels the dependence of the scale factor κ in Eq. (D.21). Therefore,

$$\frac{\Omega}{L^2} = -\frac{m\mu^2}{8\pi\hbar^2}\ln\left(\frac{4\hbar^2}{e^{2\gamma+1/2}ma^2\mu}\right), \tag{D.24}$$

This grand-canonical potential is also calculated by means of the convergence-factor regularization (CFR) [82], with the same result. On the other hand, this result agrees with that obtained in Refs. [80, 166].

The procedure outlined above we can extended to the two-dimensional Bose-Bose gas. In analogy with (D.21) we have

$$\frac{\Omega_{\mathrm{GF}}}{L^2} = -\frac{m}{8\pi\hbar^2}\sum_{\pm} f_{\pm}^2 \ln\left(\frac{\hbar^2\kappa^2}{\sqrt{e}mf_{\pm}}\right) \tag{D.25}$$

with $f_{\pm}$ given in Eq. (1.16). In this work we focused where the intra-species are equal $g_{11} = g_{22} \equiv g$. Here it is also natural to take $n_1 = n_2 \equiv n/2$, so $\mu_1 = \mu_2 \equiv \mu$. Therefore,

$$\frac{\Omega}{L^2} = -\frac{\mu^2}{g+g_{12}} - \frac{m\mu^2}{8\pi\hbar^2}\ln\left(\frac{\hbar^2\kappa^2}{\sqrt{e}m\mu}\right) - \frac{m\lambda^2\mu^2}{8\pi\hbar^2}\ln\left(\frac{\hbar^2\kappa^2}{\sqrt{e}m\lambda\mu}\right). \tag{D.26}$$

To see the independence of Ω/L^2 on the scale parameter κ we have [24, 163, 164]

$$\kappa^2\frac{\partial\Omega}{\partial\kappa^2} = 0, \qquad \to \qquad \kappa^2\frac{\partial}{\partial\kappa^2}(g+g_{12}) = \frac{m}{4\pi\hbar^2}(g^2+g_{12}^2). \tag{D.27}$$

For the one-component bosonic gas we recover the result obtained in Ref. [167].

Appendix E

Fourier transform for the dipole-dipole interaction

In this appendix we present two ways to get the Fourier transform of the dipolar term in Eq. (3.3).

E.1 First method

The dipolar interaction given in Eq. (3.3) can be written as [45, 168, 169]

$$U_{dd}\left(\mathbf{r}-\mathbf{r}'\right)=\frac{3}{4\pi}\frac{1-3\cos^2\theta}{\left|\mathbf{r}-\mathbf{r}'\right|^3}=-\frac{3}{4\pi}\left[\frac{\partial^2}{\partial z^2}\left(\frac{1}{\left|\mathbf{r}-\mathbf{r}'\right|}\right)+\frac{4\pi}{3}\delta\left(\mathbf{r}-\mathbf{r}'\right)\right]. \quad \text{(E.1)}$$

In general we have

$$u_{dd}=-\frac{\partial^2}{\partial r_i \partial r_j}\left(\frac{1}{\left|\mathbf{r}-\mathbf{r}'\right|}\right)-\frac{4\pi}{3}\delta_{ij}\delta\left(\mathbf{r}-\mathbf{r}'\right). \quad \text{(E.2)}$$

So the Fourier transform of u_{dd} given by $\tilde{u}_{dd}$ is calculated. The Fourier transform of the delta of Dira is equal to 1 . The first term is regularized as follows [94].

$$\begin{aligned}
\int d\mathbf{r}\frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{|\mathbf{r}|} &= \lim_{\epsilon\to 0}\int d\mathbf{r}\frac{e^{-\epsilon|\mathbf{r}|}}{|\mathbf{r}|}e^{-i\mathbf{k}\cdot\mathbf{r}} \\
&= 2\pi\lim_{\epsilon\to 0}\int_0^\infty dr\, re^{-\epsilon r}\int_{-1}^{1}d\left(\cos\theta\right)e^{-ikr\cos\theta} \\
&= \frac{4\pi}{k}\lim_{\epsilon\to 0}\operatorname{Im}\left(\int_0^\infty dr\, e^{-\epsilon r}e^{ikr}\right) \\
&= 4\pi\lim_{\epsilon\to 0}\frac{1}{k^2+\epsilon^2} \\
&= \frac{4\pi}{|\mathbf{k}|^2}. \qquad \text{(E.3)}
\end{aligned}$$

Since in momentum space we have $\partial/\partial r_j \rightarrow -ik_j$, the general Fourier transform of the interaction is

$$\tilde{u}\left(\mathbf{k}\right) = \sum_{ij}^{3}\left(4\pi\frac{k_i k_j}{|\mathbf{k}|^2} - \frac{4\pi}{3}\delta_{ij}\right). \tag{E.4}$$

In this work we consider the dipolar interaction with magnetization (polarization) along the z direction, so we obtain

$$\tilde{U}_{dd}\left(\mathbf{k}\right) = 3\cos^2\theta_k - 1. \tag{E.5}$$

E.2 Second method

The dipolar interaction can be written in terms of the spherical harmonics with $l = 2$ and $m = 0$, as [170]

$$U_{dd}\left(\mathbf{r}\right) = \frac{3}{4\pi r^3}\left(-4\sqrt{\frac{\pi}{5}}\right) Y_{20}\left(\theta,\phi\right). \tag{E.6}$$

Now using the expansion of a wave plane in spherical harmonics [171]

$$e^{-i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{l=0}^{\infty} i^l j_l\left(kr\right)\sum_{m=-l}^{l} Y_{lm}^{*}\left(\theta,\phi\right) Y_{lm}\left(\theta_k,\phi_k\right), \tag{E.7}$$

and the orthonormality of the spherical harmonics

$$\int d\phi\, d\theta \sin\theta\, Y_{lm}^{*}\left(\theta,\phi\right) Y_{l'm'}\left(\theta,\phi\right) = \delta_{ll'}\delta_{mm'}. \tag{E.8}$$

Thus, the Fourier transform can be written as

$$\begin{aligned}\tilde{U}_{dd}\left(\mathbf{k}\right) &= \int d\mathbf{r}\, U_{dd}\left(\mathbf{r}\right) e^{-i\mathbf{k}\cdot\mathbf{r}} \\ &= \frac{3}{4\pi}\int r^2 dr\, \sin\theta\, d\theta\, d\phi\, \frac{1}{r^3}\left(-4\sqrt{\frac{\pi}{5}}\right) Y_{20}\left(\theta,\phi\right) \\ &\times \left[4\pi\sum_{l=0}^{\infty} i^l j_l\left(kr\right)\sum_{m=-l}^{l} Y_{lm}^{*}\left(\theta,\phi\right) Y_{lm}\left(\theta_k,\phi_k\right)\right].\end{aligned} \tag{E.9}$$

The integral of the spherical Bessel function is give by

$$\begin{aligned}\int_0^\infty dr' \frac{j_2(r')}{r'} &= \int_0^\infty dr' \left(\frac{3\sin r'}{r'^4} - \frac{\sin r'}{r'^2} - \frac{3\cos r'}{r'^3}\right)\\ &= \left(-\frac{\sin r'}{r'^3} + \frac{\cos r'}{r'^2}\right)\Bigg|_0^\infty \\ &= \frac{1}{3},\end{aligned} \tag{E.10}$$

where $r' = kr$. In second line we integrate by parts twice. In the last line we also consider the expansion of the trigonometric functions for r going to 0. As $l = 2$, and $m = 0$, the only contribution to the Fourier transform in Eq. (E.9) turns out to be

$$\tilde{U}_{dd}(\mathbf{q}) = 4\sqrt{\frac{\pi}{5}} \int \sin\theta \, d\theta \, d\phi \, Y_{20}(\theta,\phi) \, Y_{20}^{*}(\theta,\phi) \, Y_{20}(\theta_q,\phi_q) \,. \tag{E.11}$$

Using the orthonormality of the spherical harmonics, Eq. (E.8), the Fourier transform of the dipolar interaction is

$$\tilde{U}_{dd}(\mathbf{k}) = 3\cos^2\theta_k - 1. \tag{E.12}$$

It is worth noting that in the literature we can find some variations of this transform, and we briefly discuss some of these situations. The numerical implementation of inverse Fourier transform of Eq. (E.12) as a part of a dipolar GPE, involves large RAM and CPU time. In particular, using split-step Crank-Nicolson method is required that using a Fourier transform continuous at the origin, on the boundary of the space discretization region both the interaction term and the wave-function should vanish. For the dipole-dipole dipole interactions this is not true, the Eq. (E.12) is discontinuous at the origin, and the boundary effects can play a role finding it. Hence a large space domain is to be used to have accurate values of this Fourier transform, involving excessive computational resources. It was suggested in Ref. [172] that this issue could be avoided by truncating the dipolar interaction conveniently at large distances $r = R$. This choice does not affect the boundary, when R is taken to be larger than the size of the condensate. In this way the truncated dipolar interaction will cover the whole condensate wave-function and a continuous Fourier transform is obtained at the origin. This method allows improve the accuracy of the calculation using a small space domain. The truncated version of the Fourier transform proposed in Ref. [172], has been numerically widely implemented, see for example Ref. [173]. This truncated Fourier transform can be obtain from Eq. (E.10) for $r = R$ instead of $r \to \infty$, so the integral can be evaluated for $0 \leq r' \leq kR$ (with $k = |\mathbf{k}|$), and we obtain

$$\tilde{U}_{dd}^{\mathrm{Trunc}}(\mathbf{k}) = (3\cos^2\theta_k - 1)\left[1 - 3\frac{\sin kR}{k^3R^3} + 3\frac{\cos kR}{k^2R^2}\right]. \tag{E.13}$$

Due to the long-range character and the anisotropy of the dipole-dipole interaction, different ways of truncating it have been considered. In Ref. [174] the aim is obtaining a mathematically well-defined Fourier transform for the dipole-dipole interaction. The main idea is to combine some elements of the two methods presented here, with suitable boundaries to the integrals. However the resulting transform, given by Eq. (85) in Ref. [174], does not allow a calculation in a closed form when the fluctuations are included. In other words, this would be a purely numerical problem. In Ref. [175] is considered a particular case explored in Ref. [174], including some physical justifications at the cost of losing a completely well mathematical definition. In this work we have chosen the Eq. (E.12), since this can be treated in closed form when we calculate the effects of the fluctuations, and at the moment it is the most used approximation. By considering the rapid development in recent years, particularly at the experimental level, the search of an improved form of the dipolar interaction remains as an open issue.

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