

QUANTUM MONTE CARLO SIMULATIONS OF ULTRACOLD ATOMIC SYSTEMS

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By
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We certify that we have read this dissertation and that in our opinion it is fully adequate, in scope and in quality, as a dissertation for the degree of Doctor of Philosophy.

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ABSTRACT

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Here, we present our work and findings on ultracold atomic systems. We first present a semi-analytical work on density wave instability (DWI) and collective modes of a bilayer dipolar system of bosons and fermions. We then show our results for quantum Monte Carlo (QMC) simulations on a bosonic system with an impurity in two-dimensions (2D). We investigate DWI on two parallel layers with antiparallel dipoles that have little to no pairing between interlayer particles. We observe that for both fermionic and bosonic bilayers, below a threshold intralayer coupling strength, no density wave instability emerges. At higher couplings, DWI forms below a critical layer spacing. We also investigate collective modes in this system. For the second problem, we present our investigations of a 2D Bose polaron, which is a system with bosonic particles and a mobile impurity. We use diffusion Monte Carlo (DMC) simulations to calculate physical quantities such as polaron energy and effective mass of the polaron as well as quantities that give insight to structural properties of the system such as pair correlation function and density profile. We model the boson-boson and boson-impurity interaction with hard spheres.

Keywords: antiparallel dipolar bilayers, density-wave instability, collective modes, Bose polaron, impurity-boson interactions, two-dimensions..

ÖZET

AŞIRI SOĞUK ATOMİK SİSTEMLERİN KUVANTUM MONTE CARLO SİMULASYONLARI

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Burada, aşırı soğuk atom sistemleri hakkındaki çalışmalarımızı sunmaktayız. Öncelikle, iki katmanlı iki kutuplu sistemin Yoğunluk Dalgası Dengesizliği ve kollektif modları ile ilgili yarı analitik işimizi sunuyoruz. Sonra, iki boyutlu (2B) saf olmayan bozonik bir sistemin Kuantum Monte Carlo simülasyonları ile ilgili işlerimizi sunuyoruz. Yoğunluk Dalgası Dengesizliğini anti paralel iki katmanlı bir sistemde, iki katman arasında çiftleşme olmadığı durumda incelemekteyiz. Hem bozon hem de fermiyonları araştırmaktayız. İki durumda da belli bir etkileşim gücünün altında yoğunluk dalgası dengesizliği gözükmediğini gözlemledik. Daha yüksek çiftleşmelerde, belli bir katmanlar arası uzaklıkta Yoğunluk Dalgası Dengesizliği oluşmakta. Ayrıca bu sistemin kollektif modlarını incelemekteyiz. Bunun dışında iki boyutlu Bozon polaron problemi konusundaki araştırmalarımızı sunmaktayız. Bu sistemde bir hareketli saf olmayan parçacık ve bozonik parçacıklar bulunmaktadır. Diffüzyon Monte Carlo yöntemi kullanarak polaron enerjisi, efektif kütle gibi fiziksel değerleri hesaplamaktayız. Aynı zamanda çift korelasyonu fonksiyonu ve yoğunluk profili gibi yapısal özellikleri de hesaplıyoruz. Bozon-bozon ve bozon-saf olmayan parçacık etkileşimini sert küre potansiyeli kullanarak modelledik.

Anahtar sözcükler: anti paralel iki kutuplu çift katman, yoğunluk dalga dengesizliği, kollektif modlar, bozon polaron, saf olmayan-bozon etkileşimi, iki boyut.

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Chapter 1

Introduction

This thesis introduces our work and findings on ultracold atomic systems. There are two major works included in the thesis, one is regarding the Density Wave Instability(DWI) of a bilayer dipole system and the other consists of Quantum Monte Carlo(QMC) simulations on a bosonic system with an impurity in 2D, also called Bose polaron in the literature.

First part of the thesis deals with the DWI instability on equal number of dipoles that are placed on a symmetric two layer structure. The moments of dipoles are aligned perpendicular to the layers. All dipoles in one layer point at the same direction and opposite to the dipoles in the other layer. We investigate both bosonic and fermionic particles in our work and assume that there is little to no pairing between the particles in different layers. We investigate formation of an inhomogeneous fluid (Density Wave) from a homogeneous superfluid by looking at the poles of the static density-density response function.

In the second part, we investigate a 2D system with bosonic particles and an impurity in an ultracold setting. The impurity acts as a polaron in this system, due to the strong interaction between itself and the bosons. We model the boson-boson interactions and impurity-boson interaction using a hard sphere potentials. We use different scattering lengths for the impurity-boson interaction

to investigate the effect of the interaction strength on the system. We use diffusion Monte Carlo(DMC) simulations to calculate physical quantities such as polaron energy and effective mass of the polaron as well as functions that give insight to structural properties of the system such as pair correlation function and density profile.

Rest of the thesis is structured as follows:

The second chapter contains information about our work in DWI in which we briefly introduce the concept to the reader, inform the reader about density-density response function and the effective interactions used in the work. Then, we present our findings about DWI and collective modes of the system followed by a brief summary of the work.

In the third chapter we present our work in 2D Bose polaron problem. First, we introduce the Variational Monte Carlo(VMC) and diffusion Monte Carlo(DMC) method. Then, we introduce the system under investigation and our model. Finally, we present our results followed by a summary section.

Chapter 2

Density-wave instability and collective modes in a bilayer system of antiparallel dipoles

2.1 Introduction

In this chapter we discuss our work on Density-wave instability and collective modes in a bilayer system of antiparallel dipoles [1]. Layered structures combine interesting physics of the low-dimensional systems with the additional tunability coming from the interlayer interactions and tunneling. In condensed matter systems, several unique phenomenon such as Coulomb-drag effect [2], formation of indirect excitons and their eventual condensation [3], density wave instabilities and Wigner crystallization [4] and fractional quantum Hall effect [5, 6] in layered structures have been the subject of an immense interest in the past few decades. The isolation of graphene and other layered van der Waals materials [7] in recent years have enormously raised this enthusiasm.

Ultracold atomic and molecular systems, on the other hand, with their impressive controllability have become natural simulators of the condensed matter

and many-body theories. In particular experimental progress in trapping and cooling atoms with large magnetic moments and polar molecules, opened up a new and interesting area of exploring quantum many-body systems with large and anisotropic dipole-dipole interactions [8, 9, 10]. Bose-Einstein condensation (BEC) of polar molecules [11, 12, 13, 14], and atoms with large permanent magnetic moments [15, 16, 17] has been observed. Very recently, the droplet crystal phase of atomic dysprosium Bose-Einstein condensate have been directly observed by Kadau *et al.* [18] Dipolar fermionic gases have been cooled down near to their ground-state as well [19, 20].

In bulk geometries, the attractive part of the dipole-dipole interaction could in principle lead to instabilities, as in BEC collapse [21] or chemical reactions between particles [10]. Therefore, it is usually favorable to confine the dipolar gases into quasi-two or one-dimensional geometries, and use an external electric or magnetic field (depending on the nature of dipoles) to polarize all dipoles in the same direction. As might be expected, layered structures are also a configuration of great interest which one can tune the attractive interactions and pairing between different layers without the fear of having chemical reactions.

While the stripe or density-wave phase is naturally expected in an isolated two-dimensional (2D) system of tilted dipolar bosons [22, 23] and fermions [24, 25, 26, 27, 28, 29, 30] due to the anisotropy of the dipole-dipole interaction, this instability has been the subject of much dispute in the limit of perpendicular dipoles, where the inter-particle interaction is isotropic. While mean-field approximation [24] as well as density-functional theory (DFT) [31] and Singwi-Tosi-Land-Sjölander (STLS) [26] calculations all predict stripe phase formation at relatively low interaction strength for two-dimensional dipolar fermions, quantum Monte Carlo (QMC) simulations suggest that the stripe phase never becomes energetically favorable, up to the liquid-to-solid phase transition for perpendicular bosons [23] and fermions [32].

In double-layer structures, both bosonic and fermionic systems have attracted a lot of attention so far. The ground state properties and instabilities of fermionic bilayers have been studied within the Hartree-Fock [33, 34, 35] as well as STLS

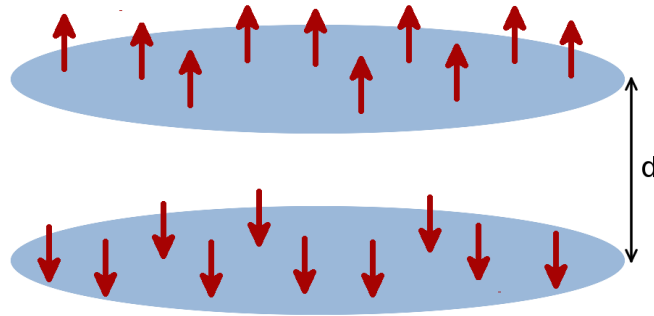


Figure 2.1: Schematic illustration of a bilayer system of dipoles with the antiparallel polarization of dipolar moments in two layers. d refers to the layer spacing between two layers.

methods [36]. The QMC simulations [37], as well as DFT calculations [38], have been employed to study the crossover from BEC to Bardeen-Cooper-Schrieffer (BCS) state too. For bosonic bilayers, on the other hand, Hufnagl and Zillich [39] have used the hypernetted-chain approximation to calculate the ground-state quantities of a bilayer system of *tilted* dipolar bosons. Then using the correlated basis function (CBF) method they obtained its dynamical properties. It has been also suggested that a bilayer system of dipolar bosons becomes a self-bound fluid when the polarization of dipoles in two layers is opposite [40]. More recently, the competition between single-dipole and dimer condensation in a bilayer of perpendicular dipolar bosons with parallel polarization, *i.e.* the same direction of polarization in both layers, have been investigated using QMC method by Macia *et al.* [41] They have observed that the pair superfluidity dominates over the single-particle superfluidity at very strong interlayer couplings, *i.e.* when the separation between two layers is much smaller than the average intralayer distance between two dipoles. The dynamical properties of the dipolar bosonic bilayer in the atomic and pair superfluid regimes have been looked at using QMC and CBF techniques [42]. The correlation effects in a bosonic bilayer have been extensively studied using QMC simulation for the ground state properties as well as the stochastic reconstruction method and method of moments for the dynamical properties by Filinov [43]

Our aim in this work is to study symmetric bilayers with the equal number of identical dipoles in each layer, whose moments are aligned perpendicular to

the 2D-planes, over a wide range of the inter-layer and intra-layer couplings. We investigate bosonic and fermionic dipolar systems on equal footing, but consider only antiparallel polarization of dipoles in two layers (see, Fig. 2.1 for a schematic illustration). Perpendicular alignment of dipoles makes both the intralayer and interlayer interactions isotropic. While the bare intralayer interaction is purely repulsive, the bare interlayer interaction could be either repulsive or attractive, depending on the in-plane separation of two dipoles. In our antiparallel configuration, the interlayer interaction is repulsive at small in-plane separations and becomes weakly attractive at large separations [see, Eqs. (2.1) and (2.2), below]. We should note that in bilayers with a parallel polarization of dipoles in two layers, the dominant interlayer interaction is attractive. At small layer spacings, this in principle leads to the pairing between dipoles of two adjacent layers. This problem has been extensively studied for both bosonic [41, 42] and fermionic systems [37, 44]. In this work, instead, our focus is on bilayers with the antiparallel polarization of dipoles. In this configuration the pairing is either absent or extremely weak [45, 46] and therefore is not expected to affect the strong interlayer screening at small layer spacings [47]. We investigate the possibility of the instability of a homogeneous fluid towards the formation of inhomogeneous densities, *i.e.* density waves. For this purpose, we look at the poles of the static density-density response function. The effective intralayer interactions are obtained from an accurate hypernetted-chain (HNC) and Fermi hypernetted-chain (FHNC) results for the static structure factor of an isolated 2D layer of bosons [48] and fermions [49], respectively, combined with the fluctuation-dissipation theorem. We have treated the interlayer interactions within the random-phase approximation (RPA) [50]. A similar study of the instability of a homogeneous liquid with respect to the inhomogeneous phase of charge density wave has been studied in a variety of quantum charged systems ranging from single-layer electron gas [51] to electron-electron and electron-hole double-layers [52, 53, 54, 55] to charged Bose systems [56] and superlattices [57, 58].

We also find semi-analytic expressions for the full dispersions of in-phase and

out-of-phase collective modes (*i.e.* zero-sound modes) from the poles of the dynamical density-density response function. For both bosonic and fermionic bilayers, the signatures of the emergence of DWI show up in the dispersions of these collective modes.

The rest of this chapter is organized as follows. In Section 2.2, we introduce the density-density response function of our system and explain how effective intralayer interaction could be obtained from the static structure factor. In Section 2.3, we look at the density wave instability for bilayer systems of dipolar bosons and dipolar fermions. In Section 2.4 we calculate the collective modes of these bilayer structures and investigate their dispersions in the vicinity of the DWI.

2.2 Density-density response function and the effective interactions

We consider two identical two-dimensional planes of dipoles, separated by the distance d . No tunneling is allowed between two layers. Therefore, layers are coupled together only through the dipole-dipole interaction. All dipoles are assumed to be polarized perpendicular to the planes, but the relative direction of this polarization is assumed to be antiparallel in two layers (see, Fig. 2.1). The bare intralayer and interlayer interactions respectively read [40]

$$V_s(r) = \frac{C_{\text{dd}}}{4\pi} \frac{1}{r^3} , \quad (2.1)$$

and

$$V_d(r) = -\frac{C_{\text{dd}}}{4\pi} \frac{r^2 - 2d^2}{(r^2 + d^2)^{5/2}} , \quad (2.2)$$

where C_{dd} is the dipole-dipole coupling constant, r is the in-plane distance between two dipoles. After Fourier transformation one finds [59, 34]

$$V_s(q) = \frac{C_{\text{dd}}}{4} \left[\frac{8}{3\sqrt{2\pi}w} - 2qe^{q^2w^2/2}\text{erfc}\left(\frac{qw}{\sqrt{2}}\right) \right] , \quad (2.3)$$

and

$$V_d(q) = \frac{C_{dd}}{2} q e^{-qd} . \quad (2.4)$$

Here $\text{erfc}(x)$ is the complementary error function and w is the short distance cut-off introduced to heal the divergence of Fourier transform of the intralayer interaction.

In this work we are interested in the density-wave instabilities and collective density modes of this double layer structure. For this we begin with the following matrix equation for the density fluctuations [50]

$$\delta n_i(\mathbf{q}, \omega) = \sum_j \chi_{ij}(\mathbf{q}, \omega) V_j^{\text{ext}}(\mathbf{q}, \omega) , \quad (2.5)$$

where $\delta n_i(\mathbf{q}, \omega)$ is the density fluctuation in layer i ($i = 1, 2$), $V_j^{\text{ext}}(\mathbf{q}, \omega)$ is the external potential applied to layer j and $\chi_{ij}(\mathbf{q}, \omega)$ is the density-density response function, whose matrix form reads

$$\hat{\chi}^{-1}(\mathbf{q}, \omega) = \hat{\Pi}^{-1}(\mathbf{q}, \omega) - \hat{W}^{\text{eff}}(\mathbf{q}, \omega) . \quad (2.6)$$

Here $\Pi_{ij}(\mathbf{q}, \omega) = \delta_{ij} \Pi_i(\mathbf{q}, \omega)$ is the non-interacting density-density response function, and $W_{ij}^{\text{eff}}(\mathbf{q}, \omega)$ is the dynamical effective potential. For symmetric bilayers we have $\Pi_i(\mathbf{q}, \omega) = \Pi(\mathbf{q}, \omega)$ (same for both layers), and $W_{ij}^{\text{eff}}(\mathbf{q}, \omega) = \delta_{ij} W_s(\mathbf{q}, \omega) + (1 - \delta_{ij}) W_d(\mathbf{q}, \omega)$, where $W_s(\mathbf{q}, \omega)$ [$W_d(\mathbf{q}, \omega)$] is the effective interaction between dipoles in the same [different] layers.

Eigenvalues of the density-density response matrix $\hat{\chi}(\mathbf{q}, \omega)$ are

$$\chi_{\pm}(\mathbf{q}, \omega) = \frac{\Pi(\mathbf{q}, \omega)}{1 - \Pi(\mathbf{q}, \omega) W_{\pm}(\mathbf{q}, \omega)} , \quad (2.7)$$

where $W_{\pm}(\mathbf{q}, \omega) = W_s(\mathbf{q}, \omega) \pm W_d(\mathbf{q}, \omega)$ are the symmetric and antisymmetric components of the effective potentials.

The non-interacting density-density response function $\Pi(\mathbf{q}, \omega)$ of a two dimensional system is analytically well known. In the case of 2D bosons, it reads

$$\Pi_B(q, \omega) = \frac{2n\varepsilon_q}{(\hbar\omega + i0^+)^2 - \varepsilon_q^2} , \quad (2.8)$$

where n is the particle density in each layer and $\varepsilon_q = \hbar^2 q^2 / (2m)$ is the single-particle energy of dipoles of mass m . The full analytic form of $\Pi(\mathbf{q}, \omega)$ for fermions is slightly more complicated and could be found *e.g.*, in Ref. [50].

The exact form of the effective potentials are not known, and one has to resort to some approximations. In the celebrated random phase approximation [50], the effective potentials are replaced with their bare values. But as the effects of exchange and correlation become more significant with increasing interaction strength, naturally the RPA which entirely discards these effects needs to be improved at strong couplings. On top of this, as the bare intralayer potential in q -space (2.3), has an artificial cut-off dependence, a simple application of RPA appears to be not very appropriate for dipolar systems even at weak couplings [35]. In order to overcome both of these problems, we use the fluctuation-dissipation theorem to find an approximate expression for the effective interlayer potential [49]. At zero temperature the fluctuation-dissipation theorem reads [50]

$$S(q) = -\frac{\hbar\pi}{n} \int_0^\infty d\omega \operatorname{Im} m \left[\frac{\Pi(q, \omega)}{1 - W_s(q, \omega)\Pi(q, \omega)} \right]. \quad (2.9)$$

Here, $S(q)$ is the static structure factor of an isolated 2D dipolar liquid, which can be obtained very accurately both for bosons and fermions *e.g.*, from QMC simulations [60, 61, 62, 32] or HNC [48] and FHNC [49] calculations. Therefore, the idea here would be to invert Eq. (2.9), and find an approximate expression for the static effective interaction in terms of the static structure factor $S(q)$. This is in principle possible if one ignores the dynamical effects, *i.e.* replaces $W_s(q, \omega)$ with a static and real function $W_s(q)$. As the effects of exchange and correlation are already included in the static structure factors, these effects will be transferred into the effective intralayer potentials, at least at the static level.

For bosons the integral over ω in Eq. (2.9) could be performed analytically, to result in

$$W_{B,s}(q) = \frac{\varepsilon_q}{2n} \left[\frac{1}{S^2(q)} - 1 \right]. \quad (2.10)$$

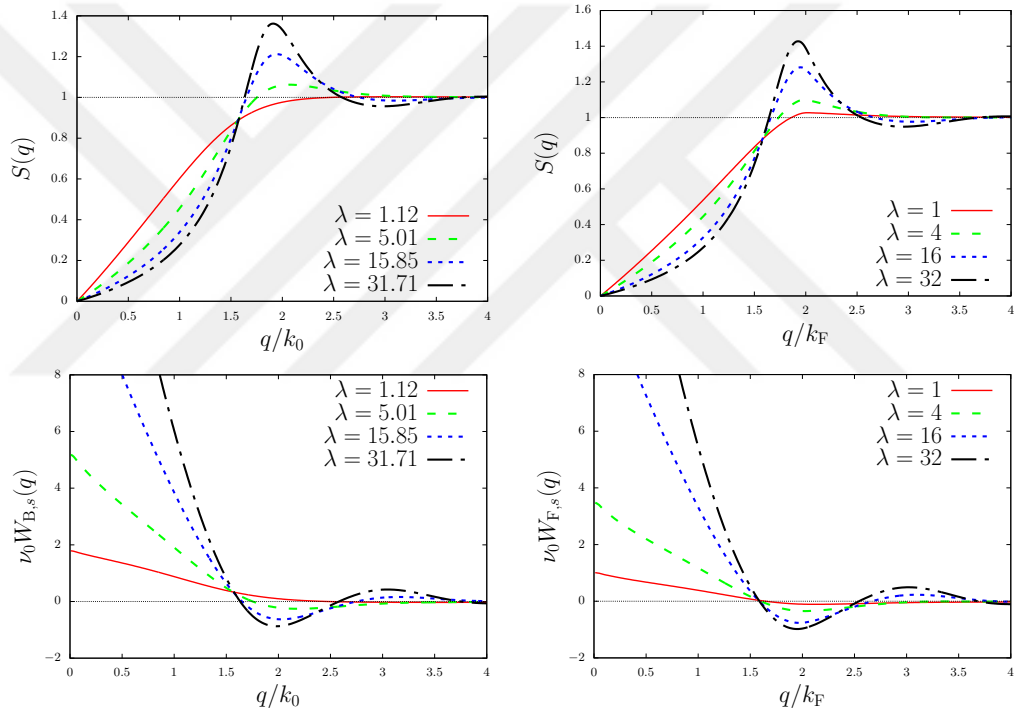


Figure 2.2: Top: static structure factor $S(q)$ of a single layer of dipolar bosons (left) and fermions (right), calculated within the HNC and FHNC formalisms, respectively. Bottom: the effective intralayer interaction of a single layer of dipolar bosons (left) and fermions (right), obtained from static structure factors and Eqs. (2.10) and (2.12), respectively.

Whereas in the fermionic case, the complicated form of the exact $\Pi(q, \omega)$ prevents an analytic solution to Eq. (2.9), however resorting to the so called “mean-spherical approximation” (MSA) for the density-density response function

$$\Pi_{\text{F}}^{(\text{MSA})}(q, \omega) = \frac{2n\varepsilon_q}{(\hbar\omega + i0^+)^2 - [\varepsilon_q/S_0(q)]^2}, \quad (2.11)$$

where $S_0(q)$ is the non-interacting static structure factor of a spin polarized 2D system of fermions [50], again an analytic solution of the frequency integral in the fluctuation-dissipation relation gives

$$W_{\text{F},s}^{(\text{MSA})}(q) = \frac{\varepsilon_q}{2n} \left[\frac{1}{S^2(q)} - \frac{1}{S_0^2(q)} \right]. \quad (2.12)$$

Note that, the MSA expressions for the non-interacting density-density response function (2.11), and the effective interaction of the fermionic system (2.12), reduce to the corresponding ones of the bosonic system with $S_0(q) \rightarrow 1$, which is indeed the correct static structure factor for non-interacting bosons.

As already mentioned, the effects of exchange and correlation, entirely ignored in the RPA, are partly included in Eqs. (2.10) and (2.12) through the interacting static structure factor $S(q)$. In Fig. 2.2 the HNC and FHNC results for the static structure factor of a single layer of dipolar bosons and fermions together with the effective intralayer interactions obtained from Eqs. (2.10) and (2.12) are illustrated for several interaction strengths λ . In the following, we set the interlayer part of the effective interaction to the bare interlayer interaction $W_d(q) = V_d(q)$, as an accurate knowledge of the interlayer static structure factors over a wide range of parameters for both bosons and fermions, is not yet available in the literature. Such an approximation is equivalent to RPA and we surmise it will be adequate for large enough layer separations.

We should note that all the properties of these bilayer systems are governed by two dimensionless parameters, namely the intralayer coupling constant $\lambda = k_0 r_0$, and the dimensionless layer spacing $k_0 d$. Here $r_0 = mC_{\text{dd}}/(4\pi\hbar^2)$ is the characteristic length scale for dipoles, and $k_0 = \sqrt{4\pi n}$. Note that k_0 is indeed the Fermi wave vector k_{F} of each layer for fermionic bilayers, but it is simply a measure of the density for bosonic bilayers.

2.3 Density-Wave Instabilities

Density-wave instabilities could be obtained from the poles of the density-density response function given in Eq. (2.7) in the static limit, or equivalently from the solution of

$$1 - \Pi(q)W_{\pm}(q) = 0 . \quad (2.13)$$

In fact, for a given system parameters such as the particle density n and layer spacing d , if Eq. (2.13) satisfies a solution with a specific wavevector q_c , then the homogenous fluid becomes unstable towards the spontaneous formation of density modulations with the wavelength $\lambda_c = 2\pi/q_c$. In the following, we investigate such an instability first for a bilayer system of dipolar bosons and then for a bilayer system of dipolar fermions.

2.3.1 Bosonic bilayers

In the static limit, the non-interacting density-density response of Eq. (2.8) reduces to

$$\Pi_B(q) = -\frac{2n}{\varepsilon_q} , \quad (2.14)$$

which together with Eq. (2.13), gives

$$1 + \frac{2n}{\varepsilon_{\mathbf{q}}} W_{B,\pm}(q) = 0 . \quad (2.15)$$

Now, using the bare interlayer potential (2.4) and the effective intralayer potential of (2.10) in Eq. (2.15) we find

$$q \pm 8\pi n r_0 S^2(q) e^{-qd} = 0 . \quad (2.16)$$

As the static structure factor is positive by definition, the above expression with positive sign will not have any solution which means that no density-wave singularity in the *in-phase* channel (*i.e.*, χ_+) appears. On the other hand, in the *out-of-phase* channel (*i.e.*, χ_-) one can find instabilities for suitable values of the interaction strength and layer spacing from the solutions of Eq. (2.16) with the

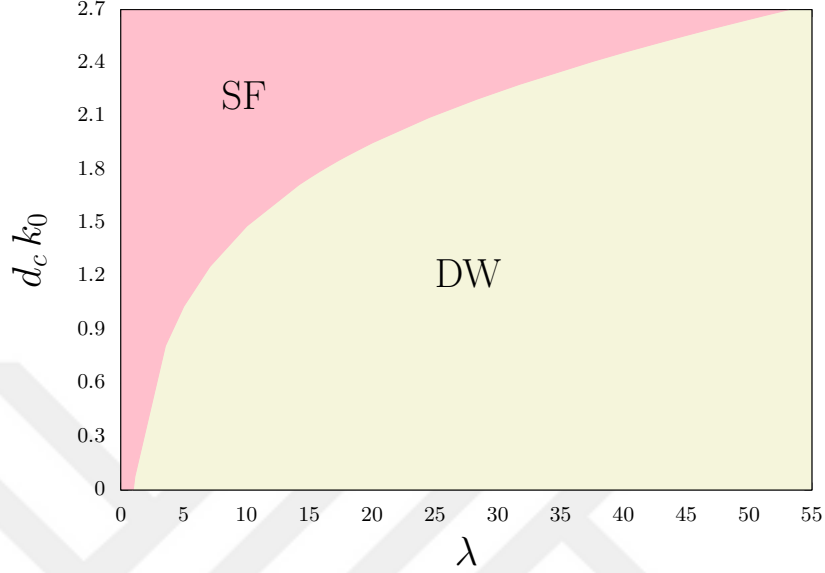


Figure 2.3: The critical layer separation d_c (in units of $1/k_0$) versus the coupling constant λ for bilayer dipolar bosons. The pink region shows the homogeneous superfluid (SF) phase and the khaki one is the region with density-wave (DW) instability.

negative sign. This means that the maxima and minima of the modulated density in two layers would be shifted by $\lambda_c/2$ with respect to each other.

Numerical investigation of Eq. (2.16) reveals that (see, Fig. 2.3) for $\lambda \gtrsim 1$ the density wave instability at a finite wave vector develops below a critical layer spacing d_c . At smaller intralayer couplings, the homogenous superfluid phase remains stable up to zero layer separations.

We note that for an isolated single layer, one has $W_d(q) = 0$, and the criteria for the density wave instability becomes

$$1 - W_s(q)\Pi(q) = \frac{1}{S^2(q)} = 0, \quad (2.17)$$

which evidently has no solution at any finite q . Therefore, within the approximations we use here, no density wave instability is expected to happen in an isolated two-dimensional system with purely repulsive dipolar interaction. In agreement with the QMC findings [23].

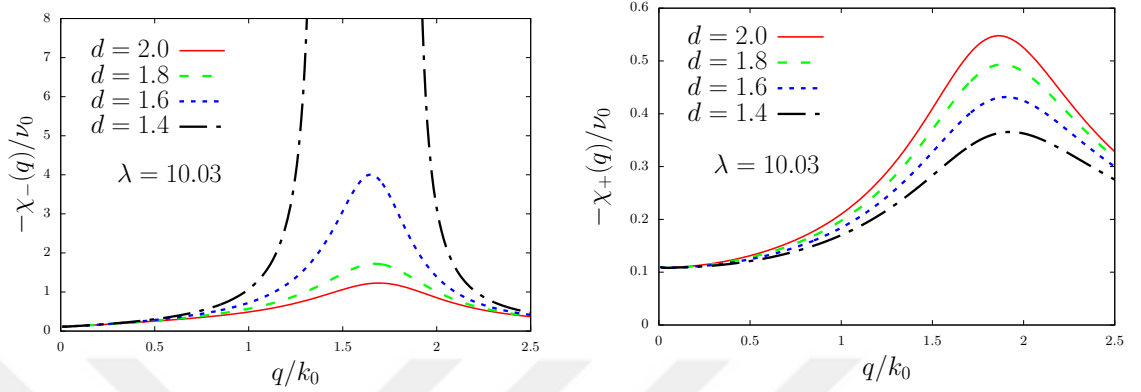


Figure 2.4: Left: The antisymmetric component of the static density-density response function $\chi_{-}(q)$ of a bilayer system of dipolar bosons, as a function of the dimensionless wave vector q/k_0 at a fixed value of the coupling constant $\lambda = 10.03$, and for several values of the layer spacing d (in units of $1/k_0$). As d approaches the critical spacing d_c , a singularity at finite q emerges in the antisymmetric component of the static density-density response function. Right: Same as the left panel but for the symmetric component of the static density-density response function $\chi_{+}(q)$.

The behavior of static density-density response functions

$$\chi_{\pm}(q) = -\nu_0 \frac{2k_0^2}{q^2/S^2(q) \pm 2\lambda k_0 q e^{-qd}} , \quad (2.18)$$

of dipolar bosons, where $\nu_0 = m/(2\pi\hbar^2)$ is the density of states per unit area of a single component 2D system, are also illustrated in Fig. 2.4 for a fixed value of the coupling constant λ and for several values of the layer spacing d . As the layer separation is lowered to the critical distance, a singularity in $\chi_{-}(q)$ emerges, but the symmetric component of the density-density response function $\chi_{+}(q)$, remains finite.

2.3.2 Fermionic bilayers

The non-interacting density-density response function of a 2D system of fermions in the static limit is [50]

$$\Pi_F(q) = -\nu_0 \left[1 - \Theta(q - 2k_F) \sqrt{1 - \left(\frac{2k_F}{q} \right)^2} \right] , \quad (2.19)$$

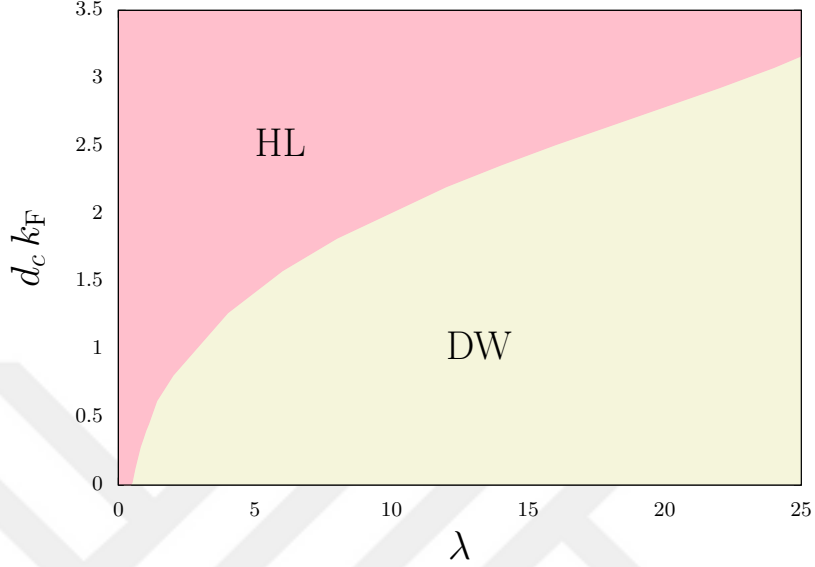


Figure 2.5: The critical layer separation d_c (in units of $1/k_F$) versus coupling constant λ for a bilayer of dipolar fermions. The pink region shows the homogeneous liquid (HL) phase and the khaki one is the region with density-wave (DW) instability.

where $k_F = k_0$ is the Fermi wave vector of a single layer. Now the density-wave instabilities could be obtained from the solutions of

$$\frac{\varepsilon_q}{2n} \left[\frac{1}{S^2(q)} - \frac{1}{S_0^2(q)} \right] \pm V_d(q) - \frac{1}{\Pi_F(q)} = 0 . \quad (2.20)$$

The phase diagram in Fig. 2.5 illustrates our numerical solution of Eq. (2.20). Similar to the bosonic bilayer, instability emerges only in the *out-of-phase* channel. The main observation here is that at a fixed density, the critical layer spacing for the formation of density waves in fermionic bilayers is slightly larger than the bosonic ones, and no DWI develops at $\lambda \lesssim 0.5$.

Figure 2.6 shows the static density-density response functions of a bilayer system of fermions

$$\chi_{\pm}(q) = \frac{1}{\Pi_F^{-1}(q) - W_{F,s}(q) \mp V_d(q)} . \quad (2.21)$$

A similar behavior to the bosonic system is observed also here. The antisymmetric component signals the emergence of DWI as the layer spacing approaches its critical value.

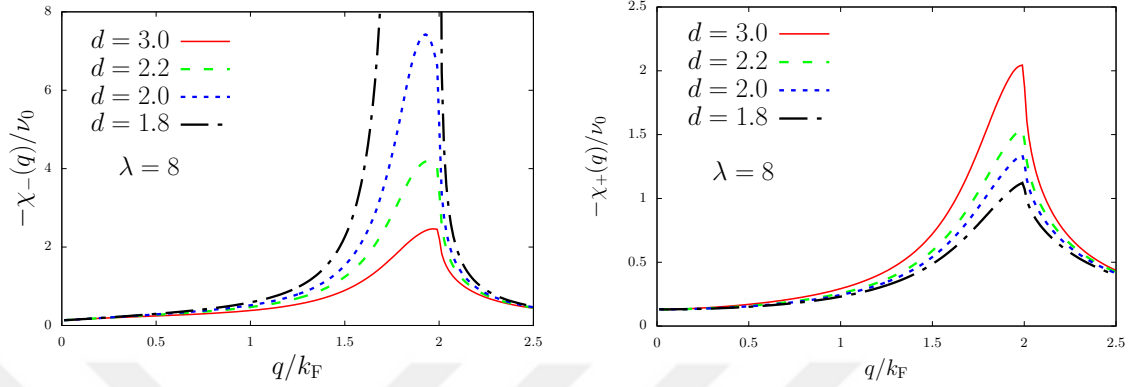


Figure 2.6: Left: The antisymmetric component of the static density-density response function $\chi_{-}(q)$ of a bilayer system of dipolar fermions, as a function of the dimensionless wave vector q/k_F for several values of the layer spacing d (in units of $1/k_F$) and at a fixed value of the coupling constant $\lambda = 8$. As d approaches the critical spacing d_c , a singularity at finite q emerges in the antisymmetric density-density response function. Right: Same as the left panel but for the symmetric component of the static density-density response function $\chi_{+}(q)$.

2.4 Collective modes

In this section, we turn to the discussion of the collective modes of dipolar bilayers. In symmetric bilayers and in the absence of tunneling between two layers, two collective density modes are simply the *in-phase* and *out-of-phase* oscillations of the particle density in two layers. The dispersion of these collective modes could be obtained from the singularities of the density-density response functions $\chi_{\pm}(q, \omega)$ at finite frequencies, or equivalently from the zeros of

$$1 - \Pi(q, \omega)W_{\pm}(q, \omega) = 0 . \quad (2.22)$$

2.4.1 Bosonic bilayers

Similar to what we did in the discussion of DWI, if we approximate the dynamical effective interaction with a static and real function, and replace the expression (2.8) for $\Pi_B(q, \omega)$ in Eq. (2.22), we will find

$$\hbar^2 \omega_{\pm}^2(q) = \varepsilon_q^2 + 2n\varepsilon_q W_{B,\pm}(q) . \quad (2.23)$$

Again, replacing the effective interlayer potential $W_d(q)$ with the bare interaction $V_d(q)$, and the effective intralayer potential $W_{B,s}(q)$ from Eq. (2.10), the dispersion of collective modes read

$$\omega_{\pm}^2(q) = \frac{\varepsilon_q}{\hbar^2} \left[\frac{\varepsilon_q}{S^2(q)} \pm nC_{dd}qe^{-qd} \right]. \quad (2.24)$$

Note that the first term on the right-hand-side of this equation is the Bijl-Feynman excitation spectrum of a single layer dipolar Bose liquid [48]. In the long-wavelength limit, as the static structure factor vanishes linearly [$S(q \rightarrow 0) \propto q$], we find

$$\omega_{\pm}(q \rightarrow 0) \approx v_{B,s}q + \mathcal{O}(q^2), \quad (2.25)$$

where $v_{B,s} = \hbar/[2mS'(0)]$ is the sound velocity of bosonic system with $S'(0) = dS(q)/dq|_{q=0}$. Unlike the charged boson bilayer [63], both collective modes of a bilayer system of dipolar bosons have acoustic nature. The reason we find same sound velocity for both collective modes relies on the fact that we are using the bare interlayer potential which vanishes linearly at small q and hence does not contribute to the sound velocity [see the second term inside the bracket in Eq. (2.24)]. One would expect deviations from this simple picture at small d , where the interlayer coupling is strong, but at larger layer spacings both sound velocities should approach the same value. Indeed, this has been verified in Ref. [40] for a bilayer of dipolar bosons with antiparallel polarization.

Using the numerical results for the static structure factor from Ref. [48] in Eq. (2.24), the full dispersions of the collective modes could be readily obtained. The results for $\omega_{\pm}(q)$ and single-layer collective mode $\omega_{sl}(q) = \varepsilon_q/[\hbar S(q)]$ are presented in Fig. 2.7 for a fixed value of the coupling constant λ and for different values of the layer separation d . We find that as the layer separation approaches the critical spacing for the density wave instability, the antisymmetric mode $\omega_{-}(q)$ touches zero and becomes soft. This occurs at the same q -value that the static density-density response function $\chi_{-}(q)$ diverges (c.f. Fig. 2.4). The energy of antisymmetric collective mode at smaller layer separations becomes negative, which is an indication of homogenous liquid phase becoming unstable.

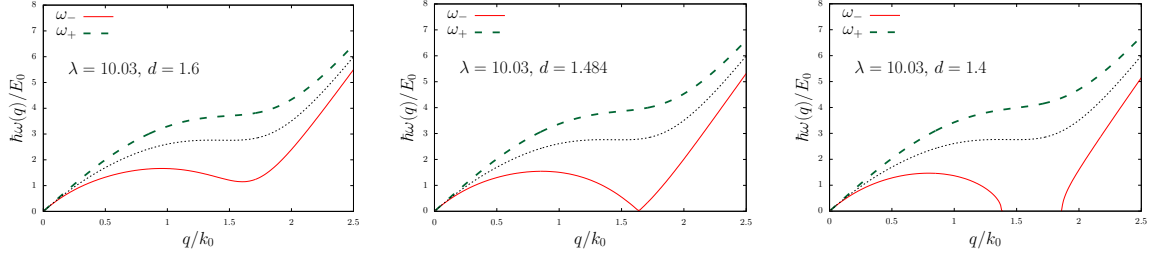


Figure 2.7: Dispersion of symmetric ω_+ and antisymmetric ω_- modes of a bilayer of dipolar bosons [in units of $E_0 = \hbar^2 k_0^2 / (2m)$], at a fixed value of the coupling constant $\lambda = 10.03$, and for different values of the layer separation: $d = 1.6/k_0$ (left), $d = 1.484/k_0$ (middle), and $d = 1.4/k_0$ (right). The dashed line represents single-layer's collective mode $\omega_{sl}(q)$. Note that $d k_0 = 1.484$ is the critical value of the layer separation for the formation of density-wave instability at $\lambda = 10.03$.

2.4.2 Fermionic bilayers

In finding the collective modes of the fermionic system, one should solve the complex equation

$$1 - W_{\pm}(q, \omega) \Pi_F(q, \omega) = 0 . \quad (2.26)$$

Again considering static effective potentials, one should search for the solutions of

$$1 - W_{\pm}(q) \operatorname{Re} e [\Pi_F(q, \omega)] = 0 , \quad (2.27)$$

outside the particle-hole continuum (PHC) *i.e.*, where $\operatorname{Im} m [\Pi_F(q, \omega)] = 0$. Using the analytic form of $\Pi_F(q, \omega)$ [50], this could be done analytically

$$\omega_{\pm}(q) = v_F q \left[1 + \frac{1}{\nu_0 W_{\pm}(q)} \right] \sqrt{\left(\frac{q}{2k_F} \right)^2 + \frac{\nu_0^2 W_{\pm}^2(q)}{1 + 2\nu_0 W_{\pm}(q)}} . \quad (2.28)$$

Here $v_F = \hbar k_F / m$ is the Fermi velocity, and this solution is valid as long as dispersions lie outside the PHC *i.e.*, $\omega_{\pm}(q) > \hbar q^2 / (2m) + v_F q$ or $0 < \omega_{\pm}(q) < \hbar q^2 / (2m) - v_F q$. In the long wavelength limit, using the fact that the fermionic static structure factors are also linear at long wavelength, and therefore the intralayer effective interaction $W_s(q)$ is finite at $q = 0$, we find

$$\omega_{\pm}(q \rightarrow 0) = v_{F,s} q + \mathcal{O}(q^2) , \quad (2.29)$$

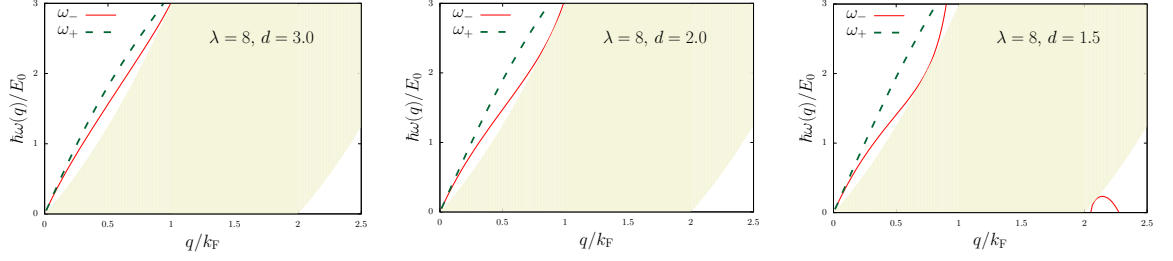


Figure 2.8: Dispersions of symmetric ω_+ and antisymmetric ω_- modes of a bilayer of dipolar fermions [in units of $E_0 = \hbar^2 k_F^2 / (2m)$] at a fixed value of the coupling constant $\lambda = 8$, and for different values of the layer separation: $d = 3.0/k_F$ (left), $d = 2.0/k_F$ (middle), and $d = 1.5/k_F$ (right). The filled areas represent the single particle excitation continuum. Note that $d = 1.82/k_F$ is the critical value of the layer separation for the formation of density-wave instability at $\lambda = 8$.

where

$$v_{F,s} = v_F \frac{1 + \nu_0 W_{F,s}(0)}{\sqrt{1 + 2\nu_0 W_{F,s}(0)}} , \quad (2.30)$$

is the fermionic sound velocity, and is related to the slopes of both interacting and noninteracting structure factors at the origin through Eq. (2.12). As $v_{F,s}$ is always larger than the Fermi velocity v_F , the zero sound waves are undamped at the long wavelength for any coupling constant and layer spacing. Interestingly, similar to the dipolar bosonic bilayers, in-phase and out-of-phase collective modes are both linear at long wavelength. Again, the degeneracy of both modes at small q should be valid only at large layer spacings. At smaller separations, the exchange-correlation effects in the effective interlayer interaction will split these two modes. Whether the lower branch will still survive the Landau damping at long wavelengths or not, requires further investigations with a more careful treatment of both intralayer and interlayer correlations.

In Fig. 2.8 we show the behavior of collective modes of the fermionic bilayer system $\omega_{\pm}(q)$ at a fixed coupling parameter λ and for different values of the layer separation. The PHC is also shown in these figures. Collective excitations are well defined only outside this continuum. Note that as the layer separation becomes smaller than the critical value (see, the right panel in Fig. 2.8), an unphysical low energy branch at $q > 2k_F$ appears below the PHC.

Chapter 3

Quantum Monte Carlo

3.1 Variational Monte Carlo

3.1.1 Variational Monte Carlo

Before explaining diffusion Monte Carlo, a general outline of the Variational Monte Carlo (VMC) system is to be given. This is necessary since the former requires the usage of the latter. For the equations and the explanation related to VMC and DMC throughout this and next sections, study of Pang [64] was used as reference.

Variational Monte Carlo is a way of approximating the ground state wavefunction using the variational principle. If we consider a quantum system with N particles, and let the positions of these particles be given by $\mathbf{R} = (r_1, r_2, \dots, r_N)$, where $r_i, i = 1, 2, \dots, N$ are the particle positions. The time independent Schrödinger equation can be written for this system as:

$$H\Psi_n(\mathbf{R}) = E_n\Psi_n(\mathbf{R}) \quad (3.1)$$

where $\Psi_n(\mathbf{R})$ are the energy eigenstates and E_n are the energy eigenvalues. Now,

variational principle gives,

$$E[\alpha_i] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi \rangle} \geq E_0 \quad (3.2)$$

for a trial wavefunction Φ . Here, E_0 is the ground state energy and α_i are any number of variational parameters. Now, the expectation value of energy can be written as,

$$E[\alpha_i] = \frac{\int \Phi^\dagger(\mathbf{R}) H \Phi(\mathbf{R}) d\mathbf{R}}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'} = \int W(\mathbf{R}) E(\mathbf{R}) d\mathbf{R} \quad (3.3)$$

and

$$W(\mathbf{R}) = \frac{|\Phi(\mathbf{R})|^2}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'}, \quad (3.4)$$

$$E(\mathbf{R}) = \frac{H\Phi(\mathbf{R})}{\Phi(\mathbf{R})}. \quad (3.5)$$

Here, $E(\mathbf{R})$ is the local energy. It corresponds to the energy of configuration $\mathbf{R}$. $W(E(\mathbf{R}))$ can be viewed as a distribution function. In the VMC scheme, one tries to variationally approximate the ground state energy by evaluating the energy of the system using (3.3) for different trial wavefunctions. In order to do achieve that, one uses the metropolis algorithm.

3.1.2 Metropolis Algorithm

Before explaining Metropolis algorithm, we first explain the detailed balance. Detailed balance is the condition that values in equilibrium satisfies the following conditions,

$$W(\mathbf{R}') T(\mathbf{R} \rightarrow \mathbf{R}') = W(\mathbf{R}) T(\mathbf{R}' \rightarrow \mathbf{R}) \quad (3.6)$$

where $T(\mathbf{R} \rightarrow \mathbf{R}')$ is the transition rate from $\mathbf{R}$ to $\mathbf{R}'$.

In the metropolis algorithm, one starts with an initial state, and then performs random walks. The resulting state after the random walk is accepted if the condition,

$$\frac{W(\mathbf{R}')}{W(\mathbf{R})} > \eta \quad (3.7)$$

where $\eta \in [0, 1]$ is a random number is satisfied, otherwise it is rejected. The accepted configurations are sampled and these samples contribute to the expectation value of the physical quantity that is calculated. This scheme, allows us to sample the system according to $W(\mathbf{R})$ and after a large number of walks we get a good enough approximation of variational energy (3.3).

3.1.3 VMC Algorithm

In this section, we explain the VMC algorithm. First, we explain the parameters of the algorithm and clarify a few points and then, we give the algorithm.

A VMC run is composed of two parts. First part is the so called thermalization part and the second part is the sampling. Number of thermalization and sampling steps are up to the user of the code, but they must be large numbers to have healthy results. We denote total number of thermalization steps as M_T and number of sampling steps as M_S . In a VMC step, each particle is applied a random walk where the particle is moved randomly in a range l . Then the new configuration is accepted or rejected according to equation 3.7. If the new configuration is accepted, then it is sampled. After the acceptance/rejection, random walk range l is adjusted so that the acceptance rate is close to %50.

1. Create N particles randomly placed in a d dimensional box.
2. For i from 0 to $M_T + M_S$,
 - (2.1) For each particle,
 - i. Move the particle using a uniformly distributed random number in range l in each dimension.
 - ii. Calculate probability of the new configuration with the moved particle according to Equation 3.4.
 - iii. Accept/reject the new configuration according to the condition in Equation 3.7.

- iv. If $i > M_T$ and the tried configuration was accepted,
 - A. Calculate and sample the desired observables of the configuration.
- v. Adjust l so that acceptance rate is closer to %50.

3.1.4 Applications

As VMC is a variational method, it can be used when the two body wavefunction is known exactly. In this case, VMC simulation gives exact results. As this is usually not the case, one of the common uses of VMC is to calculate the optimal values of variables that is included in a trial jastrow factor before a DMC or Fixed Node Monte Carlo is performed. This is vital for DMC and FN MC simulations since the trial wavefunction used in these simulations must have an overlap with the exact wavefunction of the system for the simulation to give good results.

3.1.5 Calculation of Observables

An observable A in a physical system under VMC simulation can be calculated as the average

$$\langle A \rangle = \frac{1}{M} \sum_{i=1}^M A(\mathbf{R}_i) \quad (3.8)$$

where M is the number of walkers in the current state of VMC simulation and $\mathbf{R}_i$ are the particle positions. typically at each step of the VMC simulation, the above expression is used to calculate the value of the observable.

3.2 Diffusion Monte Carlo

3.2.1 Theoretical Background for Diffusion Monte Carlo

Our aim is to develop a DMC implementation for our investigations on ultracold atomic systems. Diffusion Monte Carlo is a method for calculating the exact ground state energy of a system. The method, briefly explained, provides a method of solving the Schrödinger equation by mapping it to a diffusion equation under imaginary time transformation [64]. Now, theoretical background of DMC method will be explained.

First an imaginary time transformation is performed on many body Schrödinger equation (3.9).

$$\frac{\partial \Psi(\mathbf{R}, \tau)}{\partial \tau} = -(H - E_R)\Psi(\mathbf{R}, \tau) \quad (3.9)$$

where

$$\tau = \frac{it}{\hbar} \quad (3.10)$$

is imaginary time.

When solved, (3.9) gives,

$$\Psi(\mathbf{R}, \tau) = e^{-(H-E_R)\tau}\Psi(\mathbf{R}, 0) \quad (3.11)$$

where $\Psi(\mathbf{R}, 0)$ is the initial state. For the initial state we can choose the resulting variational wavefunction from the VMC simulation: $\Psi(\mathbf{R}, 0) = \Phi(\mathbf{R})$. From this it follows,

$$\Psi(\mathbf{R}, \tau) = \sum_n e^{-(E_n-E_R)\tau} a_n \Psi_n(\mathbf{R}) \quad (3.12)$$

where $\Psi_n(\mathbf{R})$ are the energy eigenstates and E_n are the corresponding energies. From (3.12) we see that the excited states decay faster than the ground state. At large τ , wavefunction is finite only if $E_R = E_0$.

The substitution $\Psi(\mathbf{R}, \tau) = f(\mathbf{R}, \tau)/\Phi(\mathbf{R})$ enables us to express the imaginary time Schrödinger equation as a diffusion equation:

$$\frac{\partial f(\mathbf{R}, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \nabla^2 f(\mathbf{R}, \tau) - \nabla[\mathbf{V}(\mathbf{R})f(\mathbf{R}, \tau)] - [E(\mathbf{R}) - E_R]f(\mathbf{R}, \tau) \quad (3.13)$$

where $f(\mathbf{R}, \tau) = \Phi(\mathbf{R})\Psi(\mathbf{R}, \tau)$ and $E(\mathbf{R})$ is the local energy, which denotes the current energy of the configuration $\mathbf{R}$, and

$$\mathbf{V}(\mathbf{R}) = \frac{\hbar^2}{2m} \nabla \ln |\Phi(\mathbf{R})| \quad (3.14)$$

is a term that can be interpreted as a drift velocity of the distribution in the configuration space. Time evolution of $f(\mathbf{R}, \tau)$ is given as,

$$f(\mathbf{R}', \tau + \Delta\tau) = \int G(\mathbf{R}', \mathbf{R}; \Delta\tau) f(\mathbf{R}, \tau) d\mathbf{R} \quad (3.15)$$

where,

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) = \left(\frac{1}{2\pi\chi^2} \right)^{dN/2} e^{-[\mathbf{R}' - \mathbf{R} - \Delta\tau\mathbf{V}(\mathbf{R})]^2 / 2\chi^2 - \Delta\tau[E(\mathbf{R}) - E_R]} \quad (3.16)$$

is the propagator that carries the system from $\mathbf{R}$ at time τ to $\mathbf{R}'$ at time $\tau + \Delta\tau$.

DMC algorithm makes $f(\mathbf{R}, \tau)$ evolve through τ using to the propagator given in (3.16). When the configurations are updated during the walks for the DMC simulation, three contributions from the propagator are considered.

The first and second contributions are given as,

$$\begin{aligned} \mathbf{R}' &= \mathbf{R} + \xi \\ \mathbf{R}'' &= \Delta\tau\mathbf{V}(\mathbf{R}') \end{aligned} \quad (3.17)$$

the first line applies a random walk to all particles with variance $\chi^2 = \hbar^2\Delta\tau/m$ and the second line includes a drift process that moves the mean value of the random walk applied configuration by $\Delta\tau\mathbf{V}(\mathbf{R}')$. ξ is a dN dimensional Gaussian random number with χ^2 variance, where d is the number of dimensions the physical system has.

The third contribution is a term that lowers or raises the population of configurations in the ensemble according to birth/death rate given by,

$$W_B(\mathbf{R}) \propto e^{-\Delta\tau[E(\mathbf{R}) - E_R]}. \quad (3.18)$$

This contribution is called a branching process, in which $M_B \propto W_B(\mathbf{R})$ copies of the configuration is added to the ensemble. If M_B is zero, the walker is destroyed. To control the overall number of configurations in the ensemble, reference

energy is adjusted according to the following scheme:

$$E_R \rightarrow E(\tau) + \kappa \ln \frac{N_P}{N_E} \quad (3.19)$$

where N_P is the preferred population, N_E is the current population. $E(\tau)$ is the average energy of the walkers at that instant of simulation. κ is used to control the speed of adjustment.

During a DMC simulation, the trial wavefunction from the VMC simulation $\Phi(\mathbf{R})$, evolves to the ground state of the system using the diffusion process described above. The ground state energy of the system is calculated using,

$$E(\tau) = \frac{\sum_{i=1}^{N_E} E(\mathbf{R}_i) W_B(\mathbf{R}_i)}{\sum_{i=1}^{N_E} W_B(\mathbf{R}_i)} \quad (3.20)$$

where $\mathbf{R}_i$ are the sample configurations in the ensemble.

3.2.2 Second Order Approximation

The drift applied in Eq. 3.17 is linear in $\Delta\tau$. We can further improve the algorithm by using a second order approximation. The improvement is made by replacing $\mathbf{R}'$ in the second line in Eq. 3.17 by the following expression [64]:

$$\mathbf{R}''' = \mathbf{R} + \frac{\Delta\tau}{4} \left\{ \mathbf{V}(\mathbf{R}') + \mathbf{V} \left[\mathbf{R} + \frac{\Delta\tau}{2} \mathbf{V}(\mathbf{R}) \right] \right\} \quad (3.21)$$

3.2.3 DMC Algorithm

In the DMC algorithm we start with an initial configuration that we acquire as a result of the VMC simulation. Using the propagator (3.16) given in the previous chapter, we change the configuration. The configuration then evolves through imaginary time, τ and after a sufficiently large number of time steps, it

evolves into the ground state. The algorithm stops when the fluctuations in the expected value of the physical quantity being calculated get small enough. The DMC algorithm is given as follows:

1. Create M configurations called ‘walkers’, each containing N number of particles.
2. For each walker,
 - (2.1) Apply Gaussian random walk to all particles in the walker,
 - (2.2) Apply the drift force to the walker,
 - (2.3) Calculate the branching factor M_B and do the branching,
 - (2.4) Adjust the reference energy.
3. Repeat step 2 until the desired statistical accuracy reached.

3.2.4 Parallelization

Our simulations for the homogeneous hard sphere bosons and Bose polaron systems have typically 200 walkers and 256 particles in each walker for high density and 512 particles for lower densities. As a result, simulations are computationally costly, especially for lower densities. Time required for the simulations to complete may reach up to weeks for 512 particle size.

In order to shorten the time requirements for the simulation, one may parallelize DMC steps to process and utilize more than one core at the same time. DMC can be parallelized by dividing the walkers as equally as possible into available cores. Each core will then perform the random walk, drift and then calculate the local energy of the walkers that are assigned to it. Then the processes must wait to be merged until all the processes are finished. The merging is necessary since adjustment of the reference energy requires knowledge of the number of walkers at the end of the DMC step. After all processes finish, branching is done for each walker. Branching can also be done in parallel for each process before

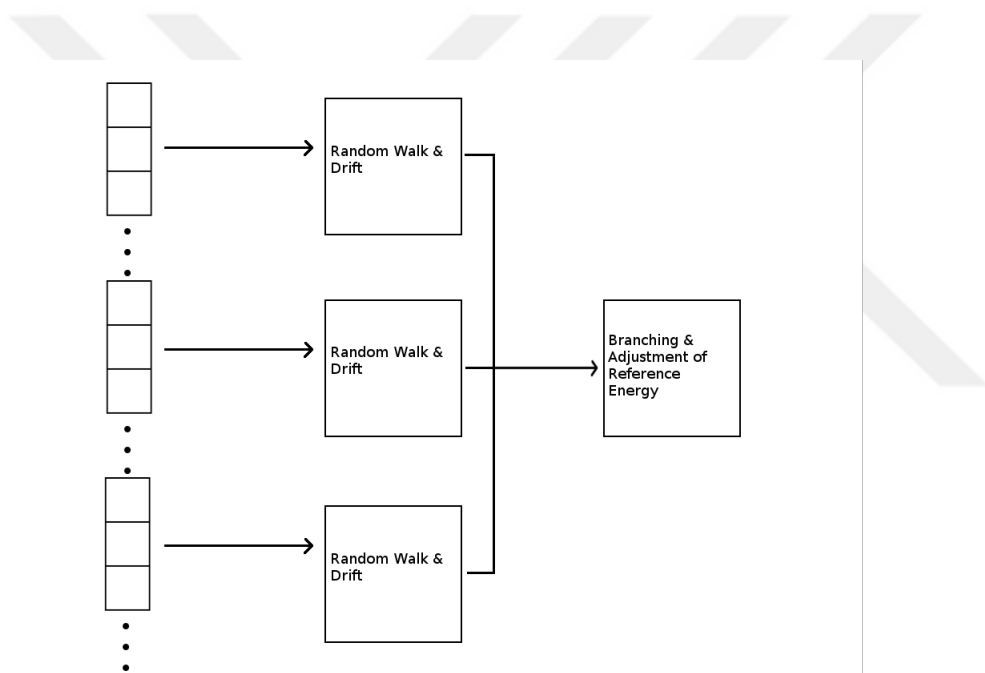


Figure 3.1: DMC is parallelized according to above scheme. First, walkers in the system are divided into number of available processes. Then random walk and drift is applied to walkers sequentially in each process. After random walk and drift is done and the energy is calculated for each process, walkers are merged and branching is done.

the merging which was not preferred in our implementation. After the branching, adjustment of the reference energy is performed.

The walkers are assigned to different processes as equally as possible. For this purpose, we divide the number of walkers in the system to number of available processes. Number of walkers assigned to each process is equal to the integer part of the result. Remaining walkers are divided into the processes until all walkers are assigned. As the number of remaining walkers is always smaller than the number of processes, each process has at most one additional walker.

3.2.5 Measured Quantities

A DMC simulation allows calculation of several different physical observables. The general idea behind the calculations is to calculate the quantity for every sample and make the necessary averaging. Some but not all the calculables are: Total energy of the system, pair correlation function, effective mass and density profile. In our work, we performed these calculations for different parameters of the system under examination.

3.2.5.1 Energy

Energy in a DMC simulation is given by,

$$E(\tau) = \frac{\sum_{i=1}^{N_E} E(\mathbf{R}_i) W_B(\mathbf{R}_i)}{\sum_{i=1}^{N_E} W_B(\mathbf{R}_i)} \quad (3.22)$$

where $\mathbf{R}_i$ are the sample configurations in the ensemble and $W_B(\mathbf{R}) = e^{-\Delta\tau[E(\mathbf{R})-E_R]}$ is the weight of the configuration. Here, N_E is the number of walkers at that instant of the simulation. The final energy value is the average of many (typically 1000 in our calculations) energy values at different imaginary

time steps calculated using the formula above. $E(\mathbf{R})$ here, is the local energy and is calculated using,

$$E(\mathbf{R}) = \frac{\hat{H}\psi(\mathbf{R})}{\psi(\mathbf{R})}. \quad (3.23)$$

for each walker.

To calculate the binding energy of the polaron, we calculate the system's energy with and without the polaron and take the difference as was done in Ardila et al.'s work [65]. The binding energy is given as,

$$E_P = E(N, 1) - E(N). \quad (3.24)$$

Here $E(N)$ is the resulting energy of the DMC simulation for bosons without the polaron and $E(N, 1)$ is the energy with the polaron.

3.2.5.2 Effective Mass

Effective mass of the impurity can be found by calculating the long term slope of the impurity displacement in imaginary time [66, 67]. It is calculated for $3D$ systems using the following expression:

$$\frac{m}{m^*} = \lim_{\tau \rightarrow \infty} \frac{\langle |\Delta \mathbf{r}_a(\tau)|^2 \rangle}{6D\tau} \quad (3.25)$$

where $D = \hbar^2/2m$ is the diffusion constant of a free particle and $\langle |\Delta \mathbf{r}_a(\tau)|^2 \rangle = \langle |\mathbf{r}_a(\tau) - \mathbf{r}_a(0)|^2 \rangle$ is the mean square displacement of the impurity in imaginary time.

For a $2D$ system, above expression must be modified slightly. The expression for effective mass calculation in $2D$ is given as below:

$$\frac{m}{m*} = \lim_{\tau \rightarrow \infty} \frac{\langle |\Delta \mathbf{r}_a(\tau)|^2 \rangle}{4D\tau} \quad (3.26)$$

which uses exactly the same variables defined for the 3D system.

3.2.5.3 Pair Correlation Function

Pair correlation function gives the probability of finding a particle at a given distance. It is defined as [68]

$$g(|\mathbf{r}_2 - \mathbf{r}_1|) = \frac{N(N-1)}{n^2} \frac{\int |\psi(\mathbf{R})|^2 dr_3 \dots dr_N}{\int |\psi(\mathbf{R})|^2 d\mathbf{R}}. \quad (3.27)$$

In order to calculate the pair correlation function in a DMC simulation, we use the method explained in Astrakharchik's work [68],

$$g^{2D}(z) = \frac{1}{\pi z h n N} \sum_{i < j} \nu_h(|\mathbf{z}_{ij} - \mathbf{z}|) \quad (3.28)$$

where $\nu_h(z)$ is 1 if $z < h$ and zero otherwise.

We also calculate the probability of finding a particle at a distance r away from an impurity. The following formula is used:

$$g_{IB}^{2D}(z) = \frac{1}{\pi z h n} \sum_{i < j} \nu_h(|\mathbf{z}_{ij} - \mathbf{z}|) \quad (3.29)$$

where $\nu_h(z)$ is 1 if $z < h$ and zero otherwise. This is same as $g_{BB}(r)$ except a factor of N .

3.2.5.4 Density Profile

Density profile is calculated by the following integral [65],

$$n(r) = n \frac{\int_0^r dr' r' g_{IB}(r')}{r^2/2}. \quad (3.30)$$

Additionally average number of particles around the impurity is found by [65],

$$N_B = 2\pi n \int_0^r dr' r' g_{IB}(r'). \quad (3.31)$$

Calculation of the above integrals are performed numerically using results of g_{IB} calculation from DMC.

Chapter 4

2D Bose Polaron Problem

4.1 Introduction

The chapter is organized as follows: The second section is devoted to the Bose polaron problem. Here, we briefly mention the concept of polaron and Bose polaron then move on to experimental and theoretical work in this field. In the third section, we present the model we used in our work and we formulate the 2D Bose polaron problem. In the third chapter, we provide the results of our work. The final chapter consists of our comments and remarks about our work.

4.2 Bose Polaron Problem

4.2.1 Early History

A polaron is a quasiparticle that distorts its environment as it moves through a medium and this distortion generally causes a significant modification in its motion. Earliest studies on this concept was from Landau and Pekar [69, 70], Fröhlich [71] and Holstein [72, 73]. They showed that an electron can distort

the ionic lattice around it; causes its motion to be modified and changes its effective mass. This effect can be understood, qualitatively by considering an electron moving with a cloud of phonons [74]. About 30 years ago polarons and bipolarons came to the fore in the context of high critical temperature (high-T_c) superconductivity [75, 76, 77] and they were instrumental in our understanding of various many-body systems such as organic superconductors and heavy-fermion superconductors.

We are interested in the Bose polaron problem, where a mobile impurity is immersed in a BEC and acts as a polaron. Earlier works studied the Fermi polaron in detail which is an impurity surrounded by fermionic atoms. [78] New experiments (our main motivation for this work) used Bose condensed gases and an impurity atom therefore the quasiparticles forming in these new systems are called Bose polarons. In order to familiarize the reader with the subject and the current literature, we will briefly mention several experimental and theoretical works in this field in the rest of this section.

4.2.2 Experimental Realizations of the Bose Polaron Problem

There has been some experimental realizations of impurities interacting with BEC. Ospelkaus et al. observed a localized phase of bosonic atoms by fermionic impurities in a 3D optical lattice [79]. Schmid et al. studied the dynamics of a trapped ion (Ba^+ or Rb^+) with an optically trapped BEC of ^{87}Rb atoms [80]. Zipkes et al. prepared a single trapped ion ($^{174}\text{Yb}^+$) in a trapped BEC of ^{87}Rb atoms [81]. Spethmann et al. doped single Cs atoms in an ultracold uncondensed Rb gas [82]. Balewski et al. study a single electron localized by a single charged ionic core immersed in a BEC of ^{87}Rb atoms [83]. Scelle et al. use fermionic ^6Li confined in a 1D lattice potential immersed in a BEC of ^{23}Na atoms [84]. Marti et al. studied properties of magnons in a ferromagnetic spinor BEC of ^{87}Rb atoms [85]. These realizations investigated different properties of impurities interacting with the BEC but they didn't achieve a complete realization of the Bose polaron

system.

In 2016, two groups made experimental observations on mobile impurities immersed in a BEC, realizing the Bose polaron. These groups achieved the task by employing two different methods. Jorgensen et al. [86] prepared a trapped BEC of ^{39}K atoms and used a radio frequency (rf) pulse, which changed the spin state of a small fraction of atoms from $|1, -1\rangle$ to $|1, 0\rangle$. These atoms acted as mobile impurities in the condensate. They measured the energy of the impurity using rf spectroscopy for different interaction strengths which was tuned using a Feshbach resonance.

Hu et al., on the other hand, used fermionic ^{40}K atoms as impurities inside trapped BEC of ^{87}Rb atoms [87]. They too, used Feshbach resonance to tune the impurity-boson interaction strength and rf spectroscopy to measure the energy spectrum. These works are the first realizations of Bose polarons in the strong interaction regime.

Additional to works mentioned above, there has been experimental work on 1D systems. Dynamics of the Bose polaron was studied in 1D Bose gas by Catani et al. [88] and on a 1D lattice by Fukuhara et al. [89].

Although to our knowledge there is no realization of the Bose polaron in 2D, recently Grusdt et al. suggested an experimental setup to test the problem in a quasi-2D BEC system [74].

4.2.3 Theoretical Investigations

On the theoretical side, there has been several investigations addressing the problem. Astrakharchik et al. studied motion of a point-like impurity by solving Gross-Pitaevskii (GP) equation in a perturbative manner [90]. Self-localization was studied by Kalas et al. [91], Cucchietti et al. [92], Bruderer et al. [93], Santamore et al. [94], Blinova et al. [95] using mean field treatment and Tempere et al. [96], Novikov et al. [97] using Feynman's variational approach. Other

works further investigate the properties of the quasiparticle. T-matrix approach is used by Rath et al. [98] to calculate various quasiparticle properties and by Volosniev et al. [99] to study the behavior of a harmonically trapped system. Li et al. developed a variational approach by generalizing Chevy ansatz that is introduced for the Fermi polaron problem to study the properties of the polaron [100]. Using a perturbative approach, Christensen et al. investigated several quasiparticle properties up to third order [101]. Three body effects (i.e. Efimov effect) is studied by Levinsen et al. and shown that it lowers the energy significantly [102]. Grusdt et al. used Renormalization Group approach to analyze the problem [103]. Recently, Pastukhov investigated the properties of a Bose polaron in a dilute 2D system at low temperatures [104].

On the numerical side, Ardila et al. studied the Bose polaron system using diffusion Monte Carlo (DMC) method [65], which is a numerical calculation method that gives the exact ground state of the system. They performed DMC simulations on bosonic systems which contains one and many number of polarons to calculate quantities such as the polaron energy, effective mass and the density profile (a function that gives probability of finding a bosonic particle at a distance from the impurity) [65]. They used repulsive hard sphere potential and attractive soft well potential for impurity-boson interaction and hard sphere interaction for boson-boson interaction. Their calculations contradict other works that predict self-localization.

Further expanding the scope of their investigations, Ardila et al. performed DMC calculations on the same system with varying impurity mass values, studying the effect of mass imbalance between the impurity and the bosons on the binding energy [105].

In the case of lower dimensions, there has been a Quantum Monte Carlo study of the Bose polaron system in 1D by Parisi et al. [106]. Other theoretical work in lower dimensions includes study of self-localization in a quasi-1D BEC by Sacha et al. [107] and investigation of a driven impurity in a 1D Bose Gas by Castelnovo et al. [108].

4.3 2D Bose Polaron Problem

4.3.1 Model

The interest in the Bose polaron problem in recent years received a big impetus after its experimental realization by two groups [87, 86]. However, the problem is not so well explored in lower dimensions, especially in 2D. We are interested in the 2D Bose polaron problem hoping to find interesting physics. We use diffusion Monte Carlo simulations to investigate this system.

The same problem in 3D was studied by Ardila et al. [65]. In their work, two different kinds of impurity-boson interaction is investigated. They use repulsive hard disk (HD) and attractive soft well (SW) interaction. Hamiltonian of such a system is given below:

$$H = -\frac{\hbar^2}{2m_B} \sum_{i=1}^N \Delta_i + \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j) - \frac{\hbar^2}{2m_I} \Delta_\alpha + \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_\alpha). \quad (4.1)$$

where the first and third term are kinetic energy of bosons and impurity respectively and second and fourth terms are potential energy terms for boson-boson and boson impurity interactions. m_I is the mass of the impurity and m_B is the mass of bosons.

2D versions of the boson-boson interaction, repulsive impurity-boson interaction and attractive impurity-boson interaction potentials would be as follows:

$$V_B(r) = \begin{cases} +\infty, & r \leq a_{2D} \\ 0, & r > a_{2D} \end{cases} \quad (4.2)$$

$$V_I^R(r) = \begin{cases} +\infty, & r \leq b_{2D} \\ 0, & r > b_{2D} \end{cases} \quad (4.3)$$

where, a_{2D} is the 2D scattering length for boson-boson interaction, b_{2D} is the scattering length for impurity-boson interaction and R is the radius of the attractive soft well potential.

We are using hard disk repulsive interaction as the first step of our investigation. Our trial wavefunction is of Jastrow type with the jastrow factor given by the two body scattering solution in 2D. This form of trial wavefunction was used in Pilati et al.'s work, where the author investigates 2D homogeneous bosonic system utilizing diffusion Monte Carlo [109]. Their inquiry involves different interaction potentials. We, at least in this stage, only employ the hard disk potential solution for the two body scattering problem.

The trial wave function for the bosonic system with impurity is given by [65]:

$$\Psi_T(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{i=1}^N f_I(|\mathbf{r}_i - \mathbf{r}_\alpha|) \prod_{j < k}^N f_B(|\mathbf{r}_j - \mathbf{r}_k|) \quad (4.4)$$

here, $f_I(r)$ describes the impurity-boson interaction and $f_B(r)$ describes the boson-boson interaction and r_α is the position of the impurity. For both interactions we use Jastrow factors of the same form. The only difference between the two Jastrow factors is the scattering length (which is used to fix the constants) as the boson-boson interaction and impurity-boson interaction has different scattering lengths. The Jastrow factor is given by,

$$f_{B,I}(r) = \begin{cases} 0, & 0 < r \leq a, b \\ AJ_0(kr) + BY_0(kr), & a, b < r < d \\ 1, & r \geq d \end{cases} \quad (4.5)$$

which is the solution to the two body problem in 2D for HD potential for $r > 0$ [109]. Here, J_0 and Y_0 are Bessel functions. The constants can be fixed by imposing the boundary conditions: $f(r \leq a_{2D}) = 0$ (for boson-boson interaction), $f(r \leq b_{2D}) = 0$ (for impurity-boson interaction), $f(r \geq d) = 1$, $f'(r \geq d) = 0$ where d is left as a variational parameter and is claimed to give an optimal result when $d = L/2$ [109]. The last constraint for the jastrow factor is that only one node is allowed for $a_{2D} \leq r \leq d$ (or $b_{2D} \leq r \leq d$ for impurity-boson interaction). We have also employed the following Jastrow factor

$$f_{B,I}(r) = \begin{cases} 0, & 0 < r \leq a, b \\ C \ln(r/(a \text{ or } b)), & a, b < r < d \\ 1, & r \geq d \end{cases} \quad (4.6)$$

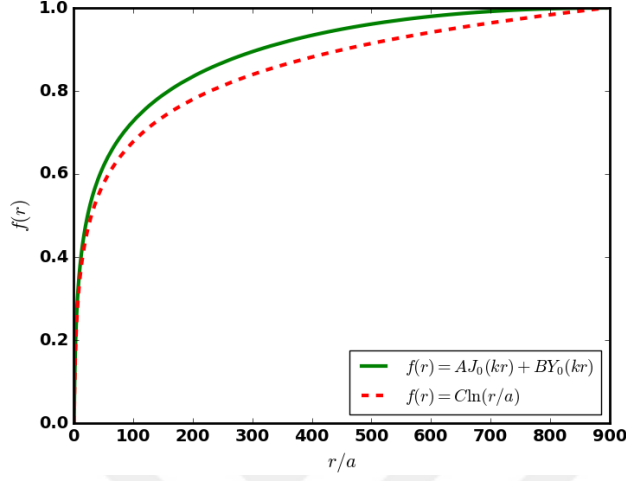


Figure 4.1: Jastrow factors for two models of hard-core interaction used in simulations as a function of r/a for $r \leq L/2$ and $na^2 = 10^{-5}$.

in which C is a constant determined by similar conditions above. This latter form is motivated by the recent proposal of Petrov and Astrakharchick [110]. We display in Fig. 4.1 the two Jastrow factors used in this work at $na^2 = 10^{-5}$ as a function of r for $r < L/2$.

4.3.2 Perturbation Theory

We follow the treatment in Ardila et al.'s work [65] and start with the Bogoliubov Hamiltonian,

$$H_B = E_B + \sum_{\mathbf{k}} \epsilon_k \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}. \quad (4.7)$$

where E_B is the ground state energy of bosonic particles,

$$E_B = \frac{\hbar^2}{2m_B} \frac{4\pi n}{\ln(1/na^2)} N \quad (4.8)$$

and operators $\alpha_{\mathbf{k}}^\dagger, \alpha_{\mathbf{k}}$ are given by the Bogoliubov transformations,

$$\begin{aligned}\alpha_{\mathbf{k}} &= u_k a_{\mathbf{k}} - v_k a_{-\mathbf{k}}^\dagger, \\ \alpha_{\mathbf{k}}^\dagger &= u_k a_{\mathbf{k}} - v_k a_{-\mathbf{k}}^\dagger,\end{aligned}\tag{4.9}$$

with $u_k^2 = 1 + v_k^2 = \frac{\epsilon_k^0 + gn_0 + \epsilon_k}{2\epsilon_k}$ and $u_k v_k = -\frac{gn_0}{2\epsilon_k}$. ϵ_k is the Bogoliubov spectrum

$$\epsilon_k = \sqrt{(\epsilon_k^0)^2 + 2gn_0\epsilon_k^0}\tag{4.10}$$

where $\epsilon_k^0 = \frac{\hbar^2 k^2}{2m_B}$, g is the boson coupling constant given as $g = \frac{4\pi}{m_B \ln(1/na^2)}$ and n_0 is the density of condensed particles.

Interaction energy of the impurity at position $\mathbf{r}_\alpha$ with the bath at mean field level is given by,

$$H_{int} = g_{BI} \int d\mathbf{r} n(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_\alpha)\tag{4.11}$$

where $g_{BI} = -\frac{2\pi}{m_{red} \ln(1/nb^2)}$ [111] is the coupling between the impurity and bosons with m_{red} the reduced mass (i.e., $1/m_{red} = 1/m_I + 1/m_B$).

Above Hamiltonian can be written in momentum space using Bougoliubov approximation $\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}+\mathbf{q}} = \sqrt{n_0 V} (u_q + v_q)(\alpha_{\mathbf{q}} + \alpha_{-\mathbf{q}}^\dagger)$,

$$H_{int} = g_{BI} + \frac{g_{BI}}{\sqrt{V}} \sum_{\mathbf{q} \neq 0} e^{i\mathbf{q}\mathbf{r}_\alpha} \sqrt{n_0} (u_q + v_q)(\alpha_{\mathbf{q}} + \alpha_{-\mathbf{q}}^\dagger).\tag{4.12}$$

Applying perturbation theory to $H_B + H_{int}$, ground state energy of system with N bosons and one impurity is found:

$$E_0 = E_B + g_{BI}n = E_B + \frac{2\pi n \hbar^2}{m_{red} \ln\left(\frac{1}{na^2} \frac{a^2}{b^2}\right)}.\tag{4.13}$$

Polaron energy is given by,

$$E_P = E_0 - E_B = -\frac{2\pi n\hbar^2}{m_{\text{red}} \ln\left(\frac{1}{na^2} \frac{a^2}{b^2}\right)}. \quad (4.14)$$

Recent work of Pastukhov[104] extended the above expression to a higher order in perturbation theory

$$E_P = \frac{2\pi n\hbar^2}{m_{\text{red}} |\ln(nb^2)|} \left[1 - \frac{\ln |\ln(na^2)|}{|\ln(nb^2)|} + \frac{2\gamma + \ln \pi + \frac{2\alpha}{\alpha-1} \ln \frac{2\alpha}{\alpha+1}}{|\ln(nb^2)|} \right], \quad (4.15)$$

in which $\gamma = 0.57721\dots$ is the Euler-Mascheroni constant and $\alpha = m_I/m_B$.

4.4 Results and Discussion

We have carried out DMC simulations of systems of N bosons and a single impurity using periodic boundary conditions with a square simulation box whose size L is fixed by the density n and by the total number of atoms $n = N/L^2$. We performed calculations for the density parameter $na^2 = 10^{-5}$ and various values of the ratio of boson-boson and impurity-boson scattering lengths a/b . Typically the number of bosons were $N = 512$, but simulations for boson numbers up to $N = 1024$ were also performed to test the finite-size effects.

As the polaron energy is calculated by the difference in the energy of a system with N bosons with and without an impurity, we have first reproduced the ground-state energy results for a uniform 2D system of bosons. [109]

Our results for the polaron energy E_P are shown in Fig. 4.2 as a function of $-\ln(a/b)$ the ratio of boson-boson and impurity-boson scattering lengths for the density parameter $na^2 = 10^{-5}$. For simplicity we have taken the boson and impurity masses to be the same. We have employed two forms of the hard-core Jastrow factor discussed above and found that the resulting polaron energy is largely independent of our choice. The influence of strong impurity-boson interaction is evident at small values of a/b resulting in an enhanced polaron energy. We find that both the leading order perturbation theory and the recent expression

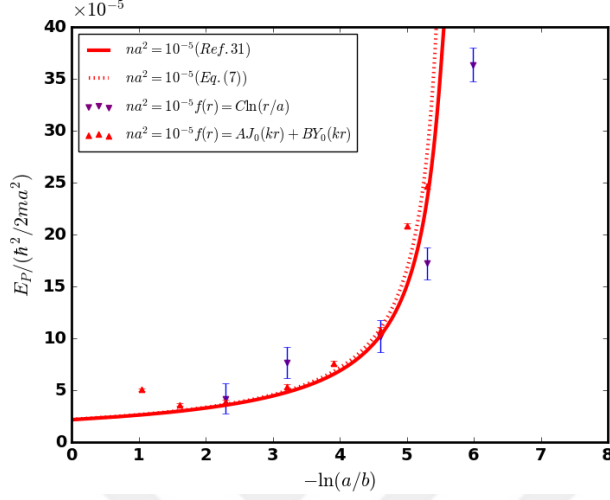


Figure 4.2: Polaron energy E_P as a function of $-\ln(a/b)$ for the density parameter $na^2 = 10^{-5}$. Error bars indicate statistical errors in the DMC simulations. Dashed and solid lines are the perturbation theory results from Eq. (7) and Eq. (8) (Ref. 31), respectively.

of Pastukhov [104] for E_P agrees with simulation results at this low value of the density parameter. However, as the density parameter na^2 is increased deviation from DMC results would become significant.

Effective mass of the impurity (polaron mass) can be found by calculating the long term slope of the mean square displacement of impurity in imaginary time [66, 67]. We have used the expression given by Eq. 3.26 for effective mass calculations of the 2D Bose polaron system.

We start the DMC simulation for effective mass calculation with 10 walkers, the same number we use for the other calculations. These 10 walkers, due to nature of the DMC algorithm multiply in size and reach around 1000 walkers. Number of time steps needed for the walker size to reach around the desired value is around 100. This value changes according to the different physical parameters of the DMC simulation (for example density, impurity-boson interaction strength, etc.) but not drastically. We make sure that this period is short relative to the total simulation time. Our simulations for this kind of procedure usually takes 1000 time steps. The convergence of the DMC algorithm is monitored by checking the

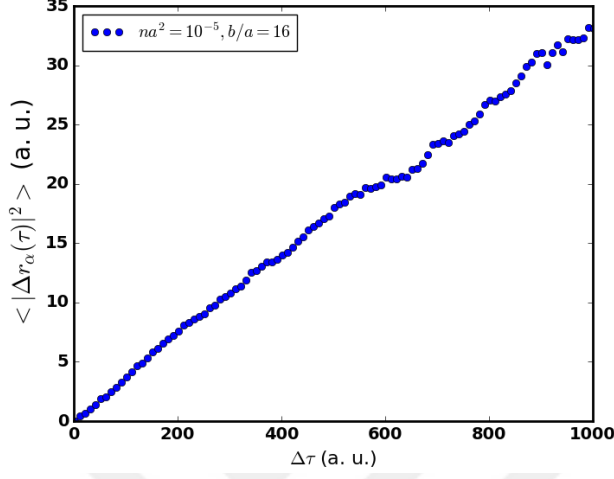


Figure 4.3: A typical mean square displacement of the impurity atom as a function of time step in arbitrary units at $na^2 = 10^{-5}$ and $b/a = 16$.

root mean square of the impurity position in imaginary time. After large enough imaginary time steps, we calculate the effective mass using the accumulated data. A data set comprises of around 1000 walkers each containing a copy of the physical system (with one impurity and usually 512 bosons) which has been subject to DMC algorithm for at least 1000 imaginary time steps. We display in Fig.4.3 a typical time evolution of mean square displacement of the impurity atom as a function of the time step $\Delta\tau$.

We have calculated the polaron effective mass at $na^2 = 10^{-5}$ as a function of $-\ln(a/b)$. The results of our calculations are shown in Fig.4.4. We find that m^*/m displays the influence of strong impurity-boson interaction at large values of b . The perturbation theory expression of Pastukhov [104]

$$\frac{m}{m^*} = 1 - \frac{1}{2\alpha} \frac{\ln(na^2)}{\ln^2(nb^2)} \quad (4.16)$$

adequately describes the trend of our simulation results.

Ardila and Giorgini[65] in their simulations of a 3D Bose gas with impurity found that m^*/m remains finite approaching the resonant point $a/b = 0$ implying the absence of self-localization. We also find an enhancement in m^*/m as $a/b \rightarrow 0$

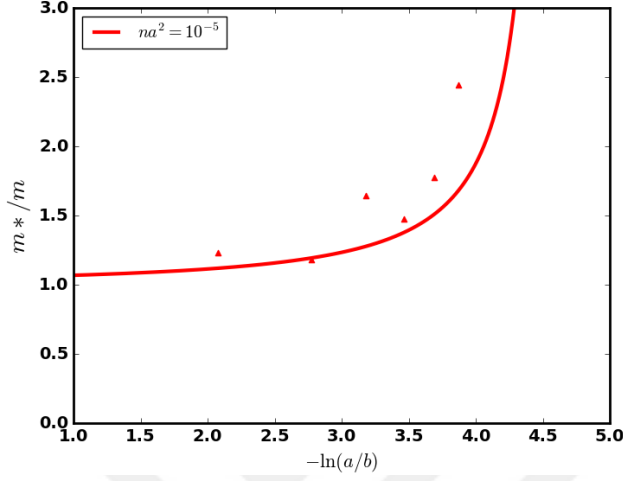


Figure 4.4: Polaron effective mass m^*/m as a function of $-\ln(a/b)$ for the density parameter $na^2 = 10^{-5}$.

but the maximum value reached depends on the density. Furthermore, for a given density parameter na^2 it becomes difficult to obtain converging results below a certain value of a/b (not shown). Whether this indicates an instability in the system or self-localization of the impurity should be investigated further.

We now turn our attention to the structural properties of the system at hand. Our first calculation is the impurity-boson pair correlation function, which gives the probability of finding a bosonic particle at a distance r from the impurity. We calculate the impurity-boson pair correlation function using Eq. 3.28.

Pair-correlation function $g_{IB}(r)$ is displayed in Fig. 4.5 for $na^2 = 10^{-5}$ and various values of b/a . Here we use the healing length in 2D $\xi = \sqrt{\ln(na^2)/n}$ [111] to scale the distance r . We find that the effect of strong impurity-boson interaction is reflected in a larger depletion at small r and a peak structure developing around $r/\xi \sim 0.8$.

The density profile of the bosons surrounding the impurity can be calculated using the expression given in Eq. 3.30.

We have calculated the integral given in Eq. 3.30 numerically using the pair

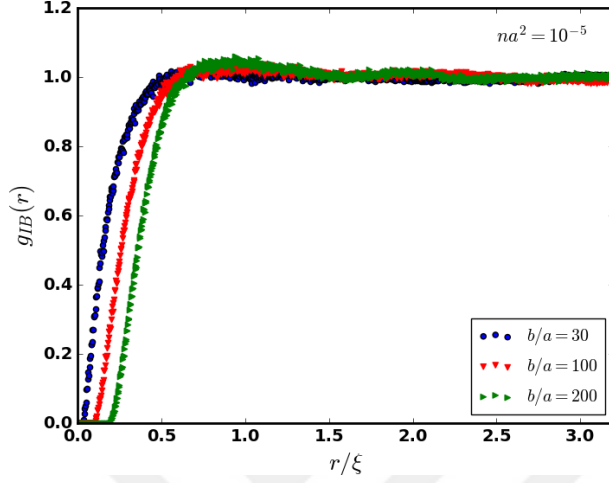


Figure 4.5: Impurity-boson pair correlation function $g_{IB}(r)$ as a function of r/ξ for $na^2 = 10^{-5}$ and different b/a values. $g_{IB}(r)$ gives the probability of finding a boson a distance r away from impurity.

correlation function $g_{IB}(r)$ from DMC simulations. Our results of $n(r)$ are shown in Fig. 4.6 as a function of r/ξ for $na^2 = 10^{-5}$ and various values of b/a . For large values of r , $n(r)$ tends to the boson density n . For small r , the strong impurity-boson repulsive interaction creates a “correlation hole” around the impurity much like the behavior in $g_{IB}(r)$. The small r behavior of $n(r)$ in 2D is different from the results of Ardila and Giorgini[65] who have found a diverging behavior for $n(r)$ as $r \rightarrow 0$ in a 3D system. The reason for this is that they use a soft-well potential with an attractive part to model the impurity-boson interaction. In our case the interaction is purely repulsive. The average number of bosons N_B surrounding the impurity is calculated by integrating the local density, $N_B = 2\pi \int_0^r dr' r' n(r')$ and shown in Fig. 4.7. We find that N_B increases with r/ξ , but the small r behavior is largely determined by the ratio b/a . For a given density na^2 , as the impurity-boson interaction increases (large b) the value of one particle ($N_B = 1$) is reached at larger values of r/ξ .

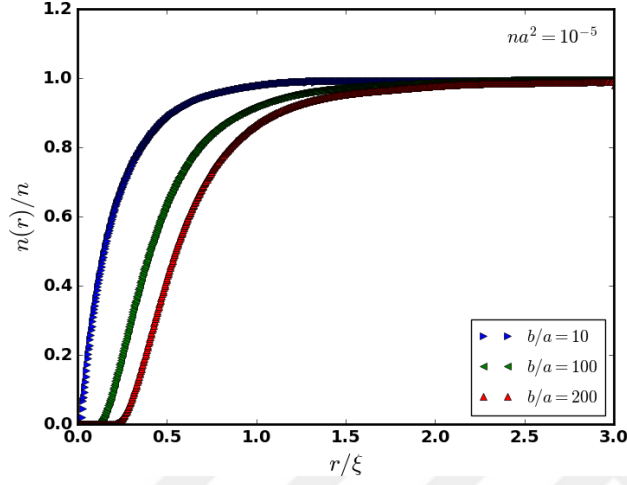


Figure 4.6: Ratio of local to uniform density of bosons $n(r)/n$ as a function of r/ξ for $na^2 = 10^{-5}$ and different b/a values.

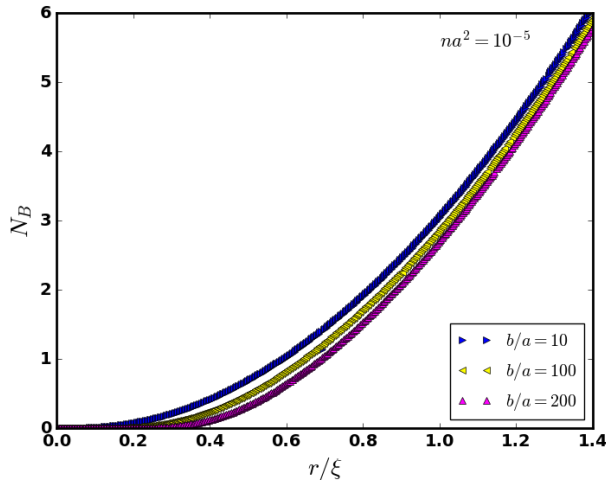


Figure 4.7: Average number of bosons N_B surrounding the impurity as a function of r/ξ for $na^2 = 10^{-5}$ and different b/a values.

Chapter 5

Conclusion

In this thesis, we discussed two different works. In the first one, we have investigated the instability of a homogenous bilayer system of perpendicular dipolar bosons and dipolar fermions with the antiparallel polarization of two layers towards density waves. Accurate HNC results for the intralayer static structure factor of bosons and FHNC results for the intralayer static structure factor of fermions are used together with the fluctuation-dissipation theorem to extract the static intralayer effective potentials and the random phase approximation is employed for the interlayer interaction. We have observed that for both fermionic and bosonic bilayers, below a threshold intralayer coupling strength λ , no density wave instability emerges. At higher couplings, DWI forms below a critical layer spacing d_c . In a given λ the DWI in fermionic bilayers sets in at a larger layer spacing in comparison with the bosonic bilayers. We have predicted that a homogenous bilayer with antiparallel polarization of dipoles in two layers is unstable towards the formation of density waves when the layer separation d becomes comparable or smaller than the average in-plane distance between particles $1/k_0$, and both of these length scales are much smaller than the dipolar length scale r_0 . We would expect this regime to be readily accessible experimentally with polar molecules whose dipolar length could easily exceed several thousands of nanometers [10].

The full dispersions of the in-phase and out-of-phase zero-sound modes of the bilayer system have been calculated too. We observed that both modes are linear at the long-wavelength limit, independent of the statistics of the particles.

Finally, we should note that in the limit of closely separated layers, improvements beyond the RPA in the effective interlayer potential, like the inclusion of exchange-correlation effects might be necessary. Dynamical effects and frequency dependence of the effective potentials would become important in the strongly correlated regime too.

In the second work, we have considered a mobile impurity in a system of bosons in 2D, all interacting repulsively, and performed QMC simulations at a very small value of the density parameter na^2 and for various values of the ratio of boson-boson and impurity-boson scattering lengths a/b . We have found that at low densities and weak impurity-boson interactions strengths perturbation theory adequately describes the polaron energy and effective mass. Our calculations discussed here may be extended in several directions. First, many impurities may be included in the simulations to study complete phase separation between the bosons and impurities, among other physical properties. Second, external trapping potentials may easily be taken into account in the simulations with appropriately chosen trial wavefunctions and Jastrow factors. Third, introducing a soft-well potential for the impurity-boson interaction may also be of interest since it would allow studying the excited states. The effects of mass difference between the impurity and bosons may also be probed. We hope our results reported here stimulates further work on Bose polarons, particularly experiments in lower dimensions.

Bibliography

- [1] E. Akaturk, S. H. Abedinpour, and B. Tanatar, “Density-wave instability and collective modes in a bilayer system of antiparallel dipoles,” *J. Phys. Commun.*, vol. 2, p. 015018, 2018.
- [2] B. N. Narozhny and A. Levchenko, “Coulomb drag,” *Rev. Mod. Phys.*, vol. 88, p. 025003, May 2016.
- [3] J. Eisenstein, “Exciton condensation in bilayer quantum hall systems,” *Annual Review of Condensed Matter Physics*, vol. 5, no. 1, pp. 159–181, 2014.
- [4] H. C. Manoharan, Y. W. Suen, M. B. Santos, and M. Shayegan, “Evidence for a bilayer quantum wigner solid,” *Phys. Rev. Lett.*, vol. 77, pp. 1813–1816, Aug 1996.
- [5] Y. W. Suen, L. W. Engel, M. B. Santos, M. Shayegan, and D. C. Tsui, “Observation of a $\nu=1/2$ fractional quantum hall state in a double-layer electron system,” *Phys. Rev. Lett.*, vol. 68, pp. 1379–1382, Mar 1992.
- [6] J. P. Eisenstein, G. S. Boebinger, L. N. Pfeiffer, K. W. West, and S. He, “New fractional quantum hall state in double-layer two-dimensional electron systems,” *Phys. Rev. Lett.*, vol. 68, pp. 1383–1386, Mar 1992.
- [7] K. S. Novoselov, A. Mishchenko, A. Carvalho, and A. H. Castro Neto, “2d materials and van der waals heterostructures,” *Science*, vol. 353, no. 6298, 2016.
- [8] M. Baranov, “Theoretical progress in many-body physics with ultracold dipolar gases,” *Physics Reports*, vol. 464, no. 3, pp. 71 – 111, 2008.

- [9] T. Lahaye, C. Menotti, L. Santos, M. Lewenstein, and T. Pfau, “The physics of dipolar bosonic quantum gases,” *Reports on Progress in Physics*, vol. 72, p. 126401, nov 2009.
- [10] M. A. Baranov, M. Dalmonte, G. Pupillo, and P. Zoller, “Condensed matter theory of dipolar quantum gases,” *Chemical Reviews*, vol. 112, pp. 5012–5061, sep 2012.
- [11] K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Pe’er, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, “A high phase-space-density gas of polar molecules,” *Science*, vol. 322, pp. 231–235, oct 2008.
- [12] K.-K. Ni, S. Ospelkaus, D. J. Nesbitt, J. Ye, and D. S. Jin, “A dipolar gas of ultracold molecules,” *Physical Chemistry Chemical Physics*, vol. 11, no. 42, p. 9626, 2009.
- [13] K.-K. Ni, S. Ospelkaus, D. Wang, G. Quémener, B. Neyenhuis, M. H. G. de Miranda, J. L. Bohn, J. Ye, and D. S. Jin, “Dipolar collisions of polar molecules in the quantum regime,” *Nature*, vol. 464, pp. 1324–1328, apr 2010.
- [14] J. Deiglmayr, A. Grochola, M. Repp, K. Mörtlbauer, C. Glück, J. Lange, O. Dulieu, R. Wester, and M. Weidemüller, “Formation of ultracold polar molecules in the rovibrational ground state,” *Phys. Rev. Lett.*, vol. 101, p. 133004, Sep 2008.
- [15] T. Lahaye, T. Koch, B. Fröhlich, M. Fattori, J. Metz, A. Griesmaier, S. Giovanazzi, and T. Pfau, “Strong dipolar effects in a quantum ferrofluid,” *Nature*, vol. 448, pp. 672–675, aug 2007.
- [16] M. Lu, N. Q. Burdick, S. H. Youn, and B. L. Lev, “Strongly dipolar bose-einstein condensate of dysprosium,” *Phys. Rev. Lett.*, vol. 107, p. 190401, Oct 2011.
- [17] K. Aikawa, A. Frisch, M. Mark, S. Baier, A. Rietzler, R. Grimm, and F. Ferlaino, “Bose-einstein condensation of erbium,” *Phys. Rev. Lett.*, vol. 108, p. 210401, May 2012.

- [18] H. Kadau, M. Schmitt, M. Wenzel, C. Wink, T. Maier, I. Ferrier-Barbut, and T. Pfau, “Observing the rosenweig instability of a quantum ferrofluid,” *Nature*, vol. 530, pp. 194–197, feb 2016.
- [19] M. Lu, N. Q. Burdick, and B. L. Lev, “Quantum degenerate dipolar fermi gas,” *Phys. Rev. Lett.*, vol. 108, p. 215301, May 2012.
- [20] J. W. Park, S. A. Will, and M. W. Zwierlein, “Ultracold dipolar gas of fermionic $^{23}\text{Na}^{40}\text{K}$ molecules in their absolute ground state,” *Phys. Rev. Lett.*, vol. 114, p. 205302, May 2015.
- [21] T. Koch, T. Lahaye, J. Metz, B. Fröhlich, A. Griesmaier, and T. Pfau, “Stabilization of a purely dipolar quantum gas against collapse,” *Nature Physics*, vol. 4, pp. 218–222, feb 2008.
- [22] A. Macia, D. Hufnagl, F. Mazzanti, J. Boronat, and R. E. Zillich, “Excitations and stripe phase formation in a two-dimensional dipolar bose gas with tilted polarization,” *Phys. Rev. Lett.*, vol. 109, p. 235307, Dec 2012.
- [23] A. Macia, J. Boronat, and F. Mazzanti, “Phase diagram of dipolar bosons in two dimensions with tilted polarization,” *Phys. Rev. A*, vol. 90, p. 061601, Dec 2014.
- [24] Y. Yamaguchi, T. Sogo, T. Ito, and T. Miyakawa, “Density-wave instability in a two-dimensional dipolar fermi gas,” *Phys. Rev. A*, vol. 82, p. 013643, Jul 2010.
- [25] K. Sun, C. Wu, and S. Das Sarma, “Spontaneous inhomogeneous phases in ultracold dipolar fermi gases,” *Phys. Rev. B*, vol. 82, p. 075105, Aug 2010.
- [26] M. M. Parish and F. M. Marchetti, “Density instabilities in a two-dimensional dipolar fermi gas,” *Phys. Rev. Lett.*, vol. 108, p. 145304, Apr 2012.
- [27] G. M. Bruun and E. Taylor, “Quantum phases of a two-dimensional dipolar fermi gas,” *Phys. Rev. Lett.*, vol. 101, p. 245301, Dec 2008.

- [28] J. K. Block and G. M. Bruun, “Properties of the density-wave phase of a two-dimensional dipolar fermi gas,” *Phys. Rev. B*, vol. 90, p. 155102, Oct 2014.
- [29] Z. Wu, J. K. Block, and G. M. Bruun, “Coexistence of density wave and superfluid order in a dipolar fermi gas,” *Phys. Rev. B*, vol. 91, p. 224504, Jun 2015.
- [30] Z. Wu, J. K. Block, and G. M. Bruun, “Liquid crystal phases of two-dimensional dipolar gases and berezinskii-kosterlitz-thouless melting,” *Scientific Reports*, vol. 6, jan 2016.
- [31] B. P. van Zyl, W. Kirkby, and W. Ferguson, “Density-functional theory for the crystalline phases of a two-dimensional dipolar fermi gas,” *Phys. Rev. A*, vol. 92, p. 023614, Aug 2015.
- [32] N. Matveeva and S. Giorgini, “Liquid and crystal phases of dipolar fermions in two dimensions,” *Phys. Rev. Lett.*, vol. 109, p. 200401, Nov 2012.
- [33] N. T. Zinner and G. M. Bruun, “Density waves in layered systems with fermionic polar molecules,” *The European Physical Journal D*, vol. 65, pp. 133–139, sep 2011.
- [34] J. K. Block, N. T. Zinner, and G. M. Bruun, “Density wave instabilities of tilted fermionic dipoles in a multilayer geometry,” *New Journal of Physics*, vol. 14, p. 105006, oct 2012.
- [35] M. Babadi and E. Demler, “Density ordering instabilities of quasi-two-dimensional fermionic polar molecules in single-layer and multilayer configurations: Exact treatment of exchange interactions,” *Phys. Rev. B*, vol. 84, p. 235124, Dec 2011.
- [36] F. M. Marchetti and M. M. Parish, “Density-wave phases of dipolar fermions in a bilayer,” *Phys. Rev. B*, vol. 87, p. 045110, Jan 2013.
- [37] N. Matveeva and S. Giorgini, “Fixed-node diffusion monte carlo study of the bcs-bec crossover in a bilayer system of fermionic dipoles,” *Phys. Rev. A*, vol. 90, p. 053620, Nov 2014.

- [38] F. Ancilotto, “Kohn-sham approach to fermi gas superfluidity: The bilayer of fermionic polar molecules,” *Phys. Rev. A*, vol. 93, p. 053627, May 2016.
- [39] D. Hufnagl and R. E. Zillich, “Stability and excitations of a bilayer of strongly correlated dipolar bosons,” *Phys. Rev. A*, vol. 87, p. 033624, Mar 2013.
- [40] M. Hebenstreit, M. Rader, and R. E. Zillich, “Dipolar bilayer with antiparallel polarization: A self-bound liquid,” *Phys. Rev. A*, vol. 93, p. 013611, Jan 2016.
- [41] A. Macia, G. E. Astrakharchik, F. Mazzanti, S. Giorgini, and J. Boronat, “Single-particle versus pair superfluidity in a bilayer system of dipolar bosons,” *Phys. Rev. A*, vol. 90, p. 043623, Oct 2014.
- [42] G. E. Astrakharchik, R. E. Zillich, F. Mazzanti, and J. Boronat, “Gapped spectrum in pair-superfluid bosons,” *Phys. Rev. A*, vol. 94, p. 063630, Dec 2016.
- [43] A. Filinov, “Correlation effects and collective excitations in bosonic bilayers: Role of quantum statistics, superfluidity, and the dimerization transition,” *Phys. Rev. A*, vol. 94, p. 013603, Jul 2016.
- [44] A. Mazloom and S. H. Abedinpour, “Superfluidity in density imbalanced bilayers of dipolar fermions,” 2017.
- [45] A. K. Fedorov, S. I. Matveenko, V. I. Yudson, and G. V. Shlyapnikov, “Novel p-wave superfluids of fermionic polar molecules,” *Scientific Reports*, vol. 6, jun 2016.
- [46] A. Boudjemâa, “Unconventional superfluids of fermionic polar molecules in a bilayer system,” *Physics Letters A*, vol. 381, pp. 1745–1748, may 2017.
- [47] A. Mazloom and S. H. Abedinpour In preparation.
- [48] S. H. Abedinpour, R. Asgari, and M. Polini, “Theory of correlations in strongly interacting fluids of two-dimensional dipolar bosons,” *Phys. Rev. A*, vol. 86, p. 043601, Oct 2012.

- [49] S. H. Abedinpour, R. Asgari, B. Tanatar, and M. Polini, “Ground-state and dynamical properties of two-dimensional dipolar fermi liquids,” *Annals of Physics*, vol. 340, pp. 25–36, jan 2014.
- [50] G. Giuliani and G. Vignale, *Quantum Theory of the Electron Liquid*. Cambridge University Press, 2008.
- [51] L. M. Sander, J. H. Rose, and H. B. Shore, “Charge-density waves in two- and three-dimensional jellium,” *Phys. Rev. B*, vol. 21, pp. 2739–2744, Apr 1980.
- [52] J. Szymański, L. Świerkowski, and D. Neilson, “Correlations in coupled layers of electrons and holes,” *Phys. Rev. B*, vol. 50, pp. 11002–11007, Oct 1994.
- [53] L. Liu, L. Świerkowski, D. Neilson, and J. Szymański, “Static and dynamic properties of coupled electron-electron and electron-hole layers,” *Phys. Rev. B*, vol. 53, pp. 7923–7931, Mar 1996.
- [54] D. Neilson, L. Świerkowski, J. Szymański, and L. Liu, “Excitations of the strongly correlated electron liquid in coupled layers,” *Phys. Rev. Lett.*, vol. 71, pp. 4035–4038, Dec 1993.
- [55] R. K. Moudgil, G. Senatore, and L. K. Saini, “Dynamic correlations in symmetric electron-electron and electron-hole bilayers,” *Phys. Rev. B*, vol. 66, p. 205316, Nov 2002.
- [56] R. K. Moudgil, P. K. Ahluwalia, and K. N. Pathak, “Ground state of a double-layer charged bose system,” *Phys. Rev. B*, vol. 56, pp. 14776–14783, Dec 1997.
- [57] A. Gold, “Instability of layered quantum liquids: 1. local-field correction in superlattices,” *Zeitschrift für Physik B Condensed Matter*, vol. 86, pp. 193–206, Jun 1992.
- [58] A. Gold, “Charge-density-wave instability in layered charged quantum liquids,” *Phys. Rev. B*, vol. 47, pp. 6762–6764, Mar 1993.

- [59] P. Lange, J. Krieg, and P. Kopietz, “Physical dipoles and second-order perturbation theory for dipolar fermions in two dimensions,” *Phys. Rev. A*, vol. 93, p. 033609, Mar 2016.
- [60] G. E. Astrakharchik, J. Boronat, I. L. Kurbakov, and Y. E. Lozovik, “Quantum phase transition in a two-dimensional system of dipoles,” *Phys. Rev. Lett.*, vol. 98, p. 060405, Feb 2007.
- [61] H. P. Büchler, E. Demler, M. Lukin, A. Micheli, N. Prokof’ev, G. Pupillo, and P. Zoller, “Strongly correlated 2d quantum phases with cold polar molecules: Controlling the shape of the interaction potential,” *Phys. Rev. Lett.*, vol. 98, p. 060404, Feb 2007.
- [62] S. Moroni and M. Boninsegni, “Coexistence, interfacial energy, and the fate of microemulsions of 2d dipolar bosons,” *Phys. Rev. Lett.*, vol. 113, p. 240407, Dec 2014.
- [63] B. Tanatar and A. K. Das, “Drag effect for a bilayer charged-bose-gas system,” *Phys. Rev. B*, vol. 54, pp. 13827–13831, Nov 1996.
- [64] T. Pang, “Diffusion monte carlo: A powerful tool for studying quantum many-body systems,” *Am. J. Phys.*, vol. 82, p. 980, 2014.
- [65] L. A. P. Ardila and S. Giorgini, “Impurity in a bose-einstein condensate: Study of the attractive and repulsive branch using quantum monte carlo methods,” *Phys. Rev. A*, vol. 92, p. 033612, 2015.
- [66] M. Boninsegni and D. M. Ceperley, “Path integral monte carlo simulation of isotopic liquid helium mixtures,” *Phys. Rev. Lett.*, vol. 74, p. 2288, 1995.
- [67] J. Boronat and J. Casulleras, “Quantum monte carlo study of static properties of one ^3He atom in superfluid ^4He ,” *Phys. Rev. B*, vol. 59, p. 8844, 1999.
- [68] G. E. Astrakharchik, “Quantum monte carlo study of ultracold gases,” *PhD Thesis, University of Trento, Italy*, 2004.
- [69] S. I. Pekar, “Local quantum states of electrons in an ideal ion crystal,” *Zh. Eksp. Teor. Fiz.*, vol. 16, p. 341, 1946.

- [70] L. D. Landau and S. I. Pekar, “Effective mass of a polaron,” *Zh. Eksp. Teor. Fiz.*, vol. 18, p. 419, 1948.
- [71] H. Frohlich, “Electrons in lattice fields,” *Advances In Physics*, vol. 3(11), p. 325, 1954.
- [72] T. Holstein, “Studies of polaron motion in the molecular-crystal model,” *Annals of Physics*, vol. 8(3), pp. 325–342, 1959.
- [73] T. Holstein, “Studies of polaron motion part (ii) the small polaron,” *Annals of Physics*, vol. 8(3), pp. 343–389, 1959.
- [74] F. Grusdt and M. Fleischhauer, “Tunable polarons of slow-light polaritons in a two-dimensional bose-einstein condensate,” *Phys. Rev. Lett.*, vol. 116, p. 053602, 2016.
- [75] N. Mott, “Polaron models of high-temperature superconductivity,” *Physica C*, vol. 205, p. 191, 1993.
- [76] S. Dzhumanov, P. Baimatov, A. Baratov, and P. Khabibullaev, “The continuum theory of delocalized and self-trapped polaron and bipolarons in solids,” *Physica C*, vol. 254, p. 311, 1995.
- [77] S. Dzhumanov, “The dependence of t_c on carrier concentration in high- t_c superconductors,” *Superlattices and Microstructures*, vol. 21, p. 363, 1997.
- [78] F. Chevy and C. Mora, “Ultra-cold polarized fermi gases,” *Rep. Prog. Phys.*, vol. 73, p. 112401, 2010.
- [79] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs, “Localization of bosonic atoms by fermionic impurities in a three-dimensional optical lattice,” *Phys. Rev. Lett.*, vol. 96, p. 180403, 2006.
- [80] S. Schmid, A. Härter, and J. H. Denschlag, “Dynamics of a cold trapped ion in a bose-einstein condensate,” *Phys. Rev. Lett.*, vol. 105, p. 133202, 2010.

- [81] C. Zipkes, S. Palzer, C. Sias, and M. Kohl, “A trapped single ion inside a bose-einstein condensate,” *Nature (London)*, vol. 464, p. 388, 2010.
- [82] N. Spethmann, F. Kindermann, S. John, C. Weber, D. Meschede, and A. Widera, “Dynamics of single neutral impurity atoms immersed in an ultracold gas,” *Phys. Rev. Lett.*, vol. 109, p. 235301, 2012.
- [83] J. B. Balewski, A. T. Krupp, A. Gaj, D. Peter, H. P. Buchler, R. Low, S. Hofferberth, and T. Pfau, “Coupling a single electron to a bose-einstein condensate,” *Nature (London)*, vol. 502, p. 664, 2013.
- [84] R. Scelle, T. Rentrop, A. Trautmann, T. Schuster, and M. K. Oberthaler, “Motional coherence of fermions immersed in a bose gas,” *Phys. Rev. Lett.*, vol. 111, p. 070401, 2013.
- [85] G. E. Marti, A. MacRae, R. Olf, S. Lourette, F. Fang, and D. M. Stamper-Kurn, “Coherent magnon optics in a ferromagnetic spinor bose-einstein condensate,” *Phys. Rev. Lett.*, vol. 113, p. 155302, 2014.
- [86] N. B. Jørgensen, L. Wacker, K. T. Skalmstang, M. M. Parish, J. Levinsen, R. S. Christensen, G. M. Bruun, and J. J. Arlt, “Observation of attractive and repulsive polarons in a bose-einstein condensate,” *Phys. Rev. Lett.*, vol. 117, p. 055302, 2016.
- [87] M.-G. Hu, M. J. V. de Graaff, D. Kedar, J. P. Corson, E. A. Cornell, and D. S. Jin, “Bose polarons in the strongly interacting regime,” *Phys. Rev. Lett.*, vol. 117, p. 055301, 2016.
- [88] J. Catani, G. Lamporesi, D. Naik, M. Gring, M. Inguscio, F. Minardi, A. Kantian, and T. Giamarchi, “Quantum dynamics of impurities in a 1d bose gas,” *Phys. Rev. A*, vol. 85, p. 023623, 2012.
- [89] T. Fukuhara, A. Kantian, M. Endres, M. Cheneau, P. Schauß, S. Hild, D. Bellem, U. Schollwöck, T. Giamarchi, C. Gross, I. Bloch, and S. Kuh, “Quantum dynamics of a mobile spin impurity,” *Nat. Phys.*, vol. 9, p. 235, 2013.

- [90] G. E. Astrakharchik and L. P. Pitaevskii, “Motion of a heavy impurity through a bose-einstein condensate,” *Phys. Rev. A*, vol. 70, p. 013608, 2004.
- [91] R. M. Kalas and D. Blume, “Interaction-induced localization of an impurity in a trapped bose-einstein condensate,” *Phys. Rev. A*, vol. 73, p. 043608, 2006.
- [92] F. M. Cucchietti and E. Timmermans, “Strong-coupling polarons in dilute gas bose-einstein condensates,” *Phys. Rev. Lett.*, vol. 96, p. 210401, 2006.
- [93] M. Bruderer, W. Bao, and D. Jaksch, “Self-trapping of impurities in bose-einstein condensates: Strong attractive and repulsive coupling,” *Europhys. Lett.*, vol. 82, p. 30004, 2008.
- [94] D. H. Santamore and E. Timmermans, “Multi-impurity polarons in a dilute bose-einstein condensate,” *New J. Phys.*, vol. 13, p. 103029, 2011.
- [95] A. A. Blinova, M. G. Boshier, and E. Timmermans, “Two polaron flavors of the bose-einstein condensate impurity,” *Phys. Rev. A*, vol. 88, p. 053610, 2013.
- [96] J. Tempere, W. Casteels, M. K. Oberthaler, S. Knoop, E. Timmermans, and J. T. Devreese, “Feynman path-integral treatment of the bec-impurity polaron,” *Phys. Rev. B*, vol. 80, p. 184504, 2009.
- [97] A. Novikov and M. Ovchinnikov, “Variational approach to the ground state of an impurity in a bose-einstein condensate,” *Phys. B*, vol. 43, p. 105301, 2010.
- [98] S. P. Rath and R. Schmidt, “Field-theoretical study of the bose polaron,” *Phys. Rev. A*, vol. 88, p. 053632, 2013.
- [99] A. G. Volosniev, H.-W. Hammer, and N. T. Zinner, “Real-time dynamics of an impurity in an ideal bose gas in a trap,” *Phys. Rev. A*, vol. 92, p. 023623, 2015.
- [100] W. Li and S. D. Sarma, “Variational study of polarons in bose-einstein condensates,” *Phys. Rev. A*, vol. 90, p. 013618, 2014.

- [101] R. S. Christensen, J. Levinsen, and G. M. Bruun, “Quasiparticle properties of a mobile impurity in a bose-einstein condensate,” *Phys. Rev. Lett.*, vol. 115, p. 160401, 2015.
- [102] J. Levinsen, M. M. Parish, and G. M. Bruun, “Impurity in a bose-einstein condensate and the efimov effect,” *Phys. Rev. Lett.*, vol. 115, p. 125302, 2015.
- [103] F. Grusdt, Y. E. Shchadilova, A. N. Rubtsov, and E. Demler, “Renormalization group approach to the fröhlich polaron model: Application to impurity-bec problem,” *Sci. Rep.*, vol. 5, p. 12124, 2015.
- [104] V. Pastukhov, “Polaron in dilute 2d bose gas at low temperatures,” *J. Phys. B: At. Mol. Opt. Phys.*, vol. 51, p. 155203, 2018.
- [105] L. A. P. Ardila and S. Giorgini, “Bose polaron problem: Effect of mass imbalance on binding energy,” *Phys. Rev. A*, vol. 94, p. 063640, 2016.
- [106] L. A. P. Ardila and S. Giorgini, “Quantum monte carlo study of the bose-polaron problem in a one-dimensional gas with contact interactions,” *Phys. Rev. A*, vol. 95, p. 023619, 2017.
- [107] K. Sacha and E. Timmermans, “Self-localized impurities embedded in a one-dimensional bose-einstein condensate and their quantum fluctuations,” *Phys. Rev. A*, vol. 73, p. 063604, 2006.
- [108] C. Castelnovo, J. S. Caux, and S. H. Simon, “Driven impurity in an ultracold one-dimensional bose gas with intermediate interaction strength,” *Phys. Rev. A*, vol. 93, p. 013613, 2016.
- [109] S. Pilati, J. Boronat, J. Casulleras, and S. Giorgini, “Quantum monte carlo simulation of a two-dimensional bose gas,” *Phys. Rev. A*, vol. 71, p. 023605, 2005.
- [110] D. Petrov and G. Astrakharchik, “Ultradilute low-dimensional liquids,” *Phys. Rev. Lett.*, vol. 117, p. 100401, 2016.
- [111] A. Posazhennikova, “Colloquium: Weakly interacting dilute bose gases in 2d,” *Rev. Mod. Phys.*, vol. 78, p. 1111, 2006.