

UNIVERSITÀ DEGLI STUDI DI TRENTO

FACOLTÀ DI SCIENZE MATEMATICHE
FISICHE E NATURALI

TESI DI LAUREA IN FISICA

Proprietà di un Gas di Bose
in Presenza di Disordine

Properties of a Bose Gas
in the Presence of Disorder

Relatori:
Dr. Stefano Giorgini
Prof. Lev P. Pitaevskii

Laureando:
Grigori Astrakhartchik

ANNO ACCADEMICO 2000-2001

Contents

Introduzione	1
Introduction	5
1 Dilute Bose gas	9
1.1 Introduction	9
1.2 Mean-field description: Gross-Pitaevskii equation	10
1.2.1 Dilute Bose gas	10
1.2.2 Gross-Pitaevskii equation	12
1.2.3 Ground state energy	13
1.2.4 Elementary excitations	14
1.3 Beyond mean-field: Bogoliubov theory	15
1.3.1 Bogoliubov Hamiltonian and elementary excitations	15
1.3.2 Ground state energy	20
1.3.3 Quantum depletion of the condensate	21
1.3.4 One-body density matrix	22
2 Dilute Bose gas with disorder: perturbation expansion	24
2.1 Introduction	24
2.2 Bogoliubov theory in the presence of disorder	25
2.2.1 Random external potential	25
2.2.2 Diagonalization of the Hamiltonian	27
2.2.3 Ground state energy	30
2.2.4 Quantum depletion of the condensate	31
2.2.5 One body density matrix	32
2.3 Superfluid density	32
2.3.1 Connection between ρ_s/ρ and the transverse current-current response function	32
2.3.2 Superfluid fraction ρ_s/ρ in the presence of disorder	36
2.3.3 calculation of the superfluid fraction from GPE	39
3 Quantum Monte Carlo Method	46
3.1 Diffusion Monte Carlo	46
3.1.1 Introduction	46
3.1.2 Schrödinger equation	47

3.1.3	Green's function	50
3.1.4	DMC algorithm	53
3.1.5	Parallel DMC algorithm	54
3.2	Homogeneous Bose Gas	56
3.2.1	Trial Wavefunction	56
3.2.2	Comparison between VMC and DMC methods	60
3.3	Outputs of the calculation	62
3.3.1	Energy	62
3.3.2	Superfluid density	63
3.3.3	One body density matrix and condensate fraction	70
3.3.4	Extrapolation technique from mixed and variational estimators	72
3.4	Systematic errors	73
3.4.1	Population of walkers	73
3.4.2	Time step	74
3.4.3	Finite size errors	74
3.4.4	Other sources of errors	76
4	Dilute Bose gas with disorder: a Diffusion Monte Carlo study	78
4.1	Introduction	78
4.2	Trial wavefunction	80
4.3	Average over disorder	83
4.3.1	Distribution of impurities	83
4.3.2	Dependence on the number of disorder realizations	84
4.4	Results	85
4.4.1	Ground-state energy	85
4.4.2	Superfluid density and condensate fraction	87
4.4.3	Scaling behaviour	91
4.4.4	Shape of the one-body density matrix	94
4.4.5	Quantum phase transition	94
	Referencies	96
A	Appendix	102
A.1	Notation for Fourier transforamtion	102
A.2	useful formulae	102
B	Series expansion of the OBDM	104
	Acknowledgements	106

Introduzione

La condensazione di Bose-Einstein (BEC) benchè proposta da Einstein [1, 2] per un gas ideale quantistico molto tempo fa (1924), rimase solo un artificio matematico fino al 1938 quando London [3] la utilizzò per spiegare la superfluidità dell' ^4He liquido. Recentemente (1995), dopo numerosi tentativi, la BEC venne osservata in una serie di esperimenti sui vapori di metalli alcalini [4, 5]. Da allora si è sviluppato notevolmente un interesse a livello mondiale per lo studio dei gas di Bose diluiti sia dal punto di vista sperimentale che teorico.

Negli ultimi anni, inoltre una grande attenzione è stata dedicata allo studio dei sistemi di Bose disordinati. La realizzazione sperimentale di questi sistemi è ottenuta per mezzo dell' assorbimento di ^4He liquido da parte di vari materiali porosi (quali *vykor* o *aerogel*). Questi sistemi mostrano varie interessanti proprietà non ancora comprese a fondo a livello teorico, quali la soppressione della superfluidità [7], la grande varietà di eccitazioni elementari [8] ed il comportamento critico, diverso da quello di *bulk*, vicino alla transizione di fase [9].

In questa tesi è stato studiato un gas di Bose in presenza di impurità fisse. Questo modello costituisce una buona approssimazione dell' ^4He liquido assorbito in materiali porosi e può diventare importante per descrivere un condensato di Bose in presenza di impurità pesanti.

A temperatura zero il sistema è descritto dai seguenti parametri:

a) na^3 (parametro del gas), dove n è la densità di particelle ed a è la lunghezza

di *scattering* in onda s .

b) $\chi = n^{imp}/n$ è la concentrazione di impurezze con una distribuzione random uniforme.

c) b/a , dove b è la lunghezza di scattering in onda s tra particella-impurezza.

Nella prima parte della Tesi si è studiato il gas di Bose diluito, trattando il potenziale esterno random in maniera perturbativa. In questo regime, utilizzando il modello di Bogoliubov, si possono ottenere analiticamente l'effetto del disordine sull'energia dello stato fondamentale, il comportamento superfluido e la componente di condensato.

Nella seconda parte della Tesi si è affrontato il problema utilizzando il metodo *Diffusion Monte Carlo* (DMC). Questo metodo numerico permette di risolvere esattamente l'equazione di Schrödinger a molti corpi per lo stato fondamentale di sistema di bosoni. Il DMC è stato utilizzato per lo studio del regime a basso disordine ed i risultati della simulazione mostrano perfetto accordo con quanto previsto dal modello di Bogoliubov. Il metodo DMC è adatto anche allo studio del regime di forte disordine. In questo regime abbiamo studiato la relazione tra il componente superfluido e la condensazione di Bose-Einstein. A bassa densità, troviamo che le componenti superfluide e condensate del sistema sono ugualmente sopresse dal disordine. Tuttavia, per concentrazioni molto alte di impurezze, troviamo che la frazione di superfluido ρ_s/ρ diviene significativamente più piccola della frazione di condensato N_0/N .

Di seguito si presenta l'organizzazione della Tesi:

Nel primo capitolo vengono riviste brevemente dapprima la teoria di campo medio di Gross-Pitaevski e la teoria di Bogoliubov per il gas di Bose diluito. Viene derivata l'equazione di Gross-Pitaevskii per il parametro d'ordine e applicata al calcolo dell'energia dello stato fondamentale del sistema. Le energie delle eccitazioni elementari sono ottenute considerando piccole oscillazioni del parametro d'ordine intorno alla soluzione d'equilibrio. Andando oltre l'approssimazione della teoria di campo

medio si è discussa l'Hamiltoniana efficace di Bogoliubov per il gas di Bose diluito. Utilizzando questo modello sono state calcolate le correzioni all'energia dello stato fondamentale, dovute alle fluttuazioni quantistiche e lo spettro di eccitazione. Discutiamo inoltre i risultati per la frazione di particelle non condensate e per la matrice densità ad un corpo.

Nel secondo capitolo è presentata la teoria del gas di Bose diluito in presenza di disordine. Utilizzando il modello di Bogoliubov si sono studiati gli effetti di un debole potenziale esterno (random), che simula la distribuzione delle impurità. Sono state calcolate la correzione all'energia dello stato fondamentale e la soppressione condensato dovuto al disordine ed il comportamento della matrice densità ad un corpo. La seconda parte del capitolo è dedicata alla definizione microscopica della densità superfluida. Usando il modello di Bogoliubov abbiamo studiato l'effetto del campo esterno sulla densità superfluida. Gli stessi risultati sono ottenuti con un nuovo metodo che fa uso dell'equazione di Gross-Pitaevskii.

Il terzo Capitolo è dedicato al metodo Monte Carlo. La tecnica DMC viene brevemente descritta e sono discusse le sue principali caratteristiche. Viene inoltre presentata l'implementazione di una versione parallela dell'algoritmo. I metodi *Diffusion Monte Carlo* (DMC) e *Variational Monte Carlo* (VMC) sono applicati ad un gas di Bose omogeneo a sfere dure: una specifica funzione di prova viene costruita e testata. Sono inoltre discusse le tecniche per il calcolo dell'energia dello stato fondamentale e la matrice densità ad un corpo. Si deriva inoltre una formula per il calcolo della densità suprefluida con l'algoritmo DMC e si mostra la sua indipendenza dalla funzione di prova. I vari tipi di errore sistematico presenti nel DMC sono studiati nell'applicazione al modello a sfere dure.

Nell'ultimo capitolo si applica il metodo DMC allo studio del gas di Bose in presenza di impurezze fisse schematizzate con sfere dure. Si prova che l'energia dello stato fondamentale di un sistema diluito $na^3 \ll 1$ nel regime di basso disordine

$\chi(b/a)^2 \ll 1$ è descritto correttamente dalle predizioni del modello di Bogoliubov. Si è studiata la dipendenza della frazione suprefluida ρ_s/ρ e della frazione di condensato N_0/N dalla densità na^3 e dai parametri di disordine χ e b/a . Abbiamo trovato che, nel limite di sistemi diluiti con debole disordine, sia ρ_s/ρ che N_0/N sono in accordo con le predizioni analitiche. Si è verificata l'esistenza di un comportamento di *scaling* in termini del parametro $R = \chi(b/a)^2$, come predetto dal modello di Bogoliubov, e si è dimostrato che questo è valido in un vasto *range* di valori di R . L'utilizzo del metodo DMC ha permesso anche di indagare il regime ad alto disordine. A basse densità e per alti valori di R abbiamo trovato che il sistema entra in un regime in cui la superfluidità viene fortemente soppressa, mentre la frazione di condensato rimane grande. È stata calcolata la dipendenza spaziale della matrice densità ad un corpo e si è mostrato l'accordo con le previsioni analitiche per basse densità. Abbiamo inoltre mostrato che la transizione quantistica da superfluido ad isolante è assente nel nostro modello di impurezze non sovrapponibili

Introduction

Although proposed by Einstein [1, 2] for an ideal quantum gas a long time ago (1924) Bose-Einstein condensation (BEC) remained only as a mathematical artifact until London “rediscovered” it in 1938 to explain the superfluidity of liquid ^4He [3]. Recently (1995), after many years of struggle, BEC was observed in alkali vapors in a remarkable series of experiments [4, 5]. Since that time there has been an explosion of experimental and theoretical interest worldwide in the study of dilute Bose gases (for a review see [6]).

In the last years great attention has been also devoted to the investigation of disordered Bose systems. The experimental realizations of these systems are liquid ^4He adsorbed in various types of porous media such as vycor and aerogel. These systems exhibit many interesting properties, which have not yet been fully understood theoretically, such as the suppression of superfluidity [7], a rich variety of elementary excitations [8] and a critical behavior near the phase transition different from the bulk [9].

In this Thesis we study a Bose gas in the presence of quenched impurities. This model provides a reasonable description of liquid ^4He adsorbed in porous media and can become relevant for Bose condensed gases in the presence of heavy impurities.

At zero temperature the system is described by the following parameters:

a) na^3 (gas parameter) where n is the density of particles na^3 and a is the s -wave scattering length,

- b) $\chi = n^{imp}/n$ is the concentration of impurities with a uniform random distribution,
- c) b/a where b is the particle-impurity s -wave scattering length

In the first part of the Thesis we investigate the dilute Bose gas by treating the random external potential as a perturbation. In this regime one can work out analytically, within the Bogoliubov model, the effect of disorder on the ground-state energy, superfluid behavior and condensate fraction.

In the second part of the Thesis we approach the problem by resorting to the Diffusion Monte Carlo (DMC) method. This numerical method solves exactly the many-body Schrödinger equation for the ground-state of a system of bosons. This method is used for the investigation of the weak disorder regime and results of the simulations agree with the predictions of the Bogoliubov model. Also the DMC method is well suited to study the regime of strong disorder. In this regime we investigate the relation between superfluid behavior and Bose-Einstein condensation. At low densities, we find that the superfluid and condensate components of the system are equally suppressed by the disorder. However, for the very large concentration of impurities, we find that the superfluid fraction ρ_s/ρ becomes significantly smaller than the condensate fraction N_0/N .

The structure of this Thesis is as follows:

In the first chapter the mean-field Gross-Pitaevskii theory and the beyond mean-field Bogoliubov theory of the dilute Bose gas are briefly reviewed. The Gross-Pitaevskii equation for the order parameter is derived and applied to the calculation of the ground-state energy of the system. The elementary excitation energies are obtained by considering the small oscillations of the order parameter around the equilibrium solution. Beyond mean-field approximation we discuss the Bogoliubov effective Hamiltonian of a dilute Bose gas and calculate within this model the excitation spectrum and corrections to the the ground-state energy arising from quantum fluctuations. The results for the fraction of noncondensed particles and the one-body

density matrix at zero temperature are also discussed.

In the second chapter we discuss the theory of a dilute Bose gas in the presence of disorder. Within the Bogoliubov model we study the effects of the weak external random potential, modeled by the uniform random distribution of quenched impurities. The corrections to the ground-state energy and the condensate depletion due to the external random potential are calculated, as well as the behavior of the one-body density matrix. The second part of this chapter is devoted to the microscopic definition of the superfluid density. By using the Bogoliubov model we investigate the effect of the external random field on the superfluid density. The same result is also obtained in a new alternative way which makes use of the Gross-Pitaevskii equation.

Chapter Three is devoted to the Quantum Monte Carlo method. The Diffusion Monte Carlo technique is briefly described and its main features are discussed. We also discuss the implementation of the parallel version of the algorithm. The Diffusion Monte Carlo (DMC) and Variational Monte Carlo (VMC) methods are applied to a hard-sphere homogeneous Bose gas, and a specific trial wave-function is constructed and tested. The techniques of calculating the ground-state energy and the one-body density matrix are presented. A formula for the calculation of the superfluid density within the DMC algorithm is derived and proved to be unbiased by the trial wave-function. All types of systematic errors present in the DMC algorithm applied to the hard-sphere model are investigated.

In the last chapter we apply the DMC method to investigate a Bose gas in the presence of hard-sphere quenched impurities. We show that the ground-state energy of a dilute system $na^3 \ll 1$ in the “weak” disorder regime $\chi(b/a)^2 \ll 1$ is described correctly by the prediction of the Bogoliubov model. We study the dependence of the superfluid fraction ρ_s/ρ and condensate fraction N_0/N on the density na^3 and disorder parameters χ and b/a . We find that in limit of dilute systems and weak disorder both ρ_s/ρ and N_0/N are in agreement with analytical predictions. The

existence of scaling in $R = \chi(b/a)^2$, as predicted by Bogoliubov model, is checked and is shown to be valid over a large range of R . The use of the DMC method enables us to investigate the regime of strong disorder. At low density and large values of R we find that the system enters a regime where the superfluid density is strongly suppressed, whereas the condensate fraction is still large. The space dependence of the one-body density matrix is calculated and is shown to agree with analytical predictions at small densities na^3 . We show that the superfluid-insulator quantum transition is absent within our model of non-overlapping impurities.

Chapter 1

Dilute Bose gas

1.1 Introduction

The present chapter is devoted to the theory of homogeneous dilute Bose gases at zero temperature.

The mean-field theory for the dilute Bose gas is discussed in the first part of the chapter. We derive the Gross-Pitaevskii equation for the order parameter and we use it to calculate the ground-state energy of the system. The small oscillations of the order parameter around the equilibrium solution provide us with the elementary excitation energies. The presentation of the material in this section follows closely the review [6].

In the second part of the chapter we discuss the Bogoliubov model, which is a theory beyond mean-field and takes into account the fluctuations of the order parameter. We introduce Bogoliubov effective Hamiltonian, discuss its diagonalization by means of the Bogoliubov transformation and we calculate the corrections to the of the ground state energy arising from the quantum fluctuations. The excitation spectrum predicted by the Bogoliubov model agrees with the one obtained from the time-dependent Gross-Pitaevskii equation. Results for the number of noncondensed

particles (quantum depletion) and the one-body density matrix are also discussed. Much of the treatment of this part of the chapter parallels closely the one given in the book [11].

1.2 Mean-field description: Gross-Pitaevskii equation

1.2.1 Dilute Bose gas

The Hamiltonian of a system of spinless bosons, interacting through the pair potential U and immersed in the external field $V(\mathbf{r})$ is given, in second quantization, by

$$\begin{aligned} \hat{H} = & \int \hat{\Psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \hat{\Psi}(\mathbf{r}) d\mathbf{r} + \\ & + \frac{1}{2} \iint \hat{\Psi}^\dagger(\mathbf{r}_2) \hat{\Psi}^\dagger(\mathbf{r}_1) U(|\mathbf{r}_1 - \mathbf{r}_2|) \hat{\Psi}(\mathbf{r}_1) \hat{\Psi}(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \end{aligned} \quad (1.1)$$

here m is the mass of a particle, $\hat{\Psi}(\mathbf{r})$ and $\hat{\Psi}^\dagger(\mathbf{r})$ are the boson field operators that annihilate and create a particle at the position \mathbf{r} .

If the gas is dilute and cold, then the two-body potential can be replaced by the pseudopotential $U(\mathbf{r}' - \mathbf{r}) = g\delta(\mathbf{r}' - \mathbf{r})$ which is fixed by a single parameter, the s -wave scattering length a , through the coupling constant

$$g = \frac{4\pi\hbar^2 a}{m} \quad (1.2)$$

The Hamiltonian (1.1) takes the form

$$\hat{H} = \int \hat{\Psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \hat{\Psi}(\mathbf{r}) d\mathbf{r} + \frac{g}{2} \iint \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) d\mathbf{r}, \quad (1.3)$$

The field operator can be decomposed as $\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r})$, where $\phi_{\mathbf{k}}(\mathbf{r})$ are single-particle wavefunctions with quantum number \mathbf{k} . The bosonic creation and annihilation operators $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}^\dagger$ are defined in Fock space through the relations

$$\hat{a}_{\mathbf{k}}^\dagger |n_0, n_1, \dots, n_k, \dots\rangle = \sqrt{n_k + 1} |n_0, n_1, \dots, n_k + 1, \dots\rangle, \quad (1.4)$$

$$\hat{a}_{\mathbf{k}} |n_0, n_1, \dots, n_k, \dots\rangle = \sqrt{n_k} |n_0, n_1, \dots, n_k - 1, \dots\rangle, \quad (1.5)$$

where n_k are the eigenvalues of the operator $\hat{n}_{\mathbf{k}} = \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}$ giving the number of atoms in the single-particle state \mathbf{k} . The operators $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}^\dagger$ obey the usual bosonic commutation rules

$$[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'}, \quad [\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}] = 0, \quad [\hat{a}_{\mathbf{k}}^\dagger, \hat{a}_{\mathbf{k}'}^\dagger] = 0. \quad (1.6)$$

Bose-Einstein condensation occurs when the number of particles in one particular single-particle state becomes very large $N_0 \gg 1$. In this limit the states with N_0 and $N_0 \pm 1 \approx N_0$ correspond to the same physical configuration and, consequently, the operators \hat{a}_0^\dagger and \hat{a}_0 can be treated as complex numbers

$$\hat{a}_0^\dagger = \hat{a}_0 = \sqrt{N_0} \quad (1.7)$$

For a uniform gas in a volume V the good single-particle states correspond to

momentum states and BEC occurs in the single-particle state $\psi_0 = 1/\sqrt{V}$ having zero momentum. Thus, the field operator $\hat{\Psi}_{\mathbf{k}}(\mathbf{r})$ can be decomposed in the form $\hat{\Psi}_{\mathbf{k}}(\mathbf{r}) = \sqrt{N_0/V} + \hat{\Psi}'(\mathbf{r})$. The generalization for the case of nonuniform and time-dependent configurations is given by

$$\hat{\Psi}_{\mathbf{k}}(\mathbf{r}, t) = \Phi(\mathbf{r}, t) + \hat{\Psi}'(\mathbf{r}, t), \quad (1.8)$$

where the Heisenberg representation for the field operators is used. Here $\Phi(\mathbf{r}, t)$ is a complex function defined as the expectation value of the field operator $\Phi(\mathbf{r}, t) = \langle \hat{\Psi}(\mathbf{r}, t) \rangle$.

The function $\Phi(\mathbf{r}, t)$ is a classical field having the meaning of an order parameter and is often called the *wave-function of the condensate*. The mean-field theory, which describes the behavior of the classical field $\Phi(\mathbf{r}, t)$ and ignores the fluctuations $\hat{\Psi}'(\mathbf{r}, t)$ is contained in the Gross-Pitaevskii theory. A more refined approach, which takes into account the fluctuations of the field operator was proposed by Bogoliubov.

1.2.2 Gross-Pitaevskii equation

In order to derive the equation for the wavefunction of the condensate $\Phi(\mathbf{r}, t)$ one has to write the time evolution of the field operator $\hat{\Psi}(\mathbf{r}, t)$ using the Heisenberg equation

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{r}, t) = [\hat{\Psi}, \hat{H}] \quad (1.9)$$

Substitution of the Hamiltonian (1.3) into (1.9) gives

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) + g|\hat{\Psi}(\mathbf{r}, t)|^2 \right) \hat{\Psi}(\mathbf{r}, t) \quad (1.10)$$

We now replace the field operator $\hat{\Psi}(\mathbf{r}, t)$ with the classical field $\Phi(\mathbf{r}, t)$. Then, the following equation for the order parameter is obtained

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) + g|\Phi(\mathbf{r}, t)|^2 \right) \Phi(\mathbf{r}, t) \quad (1.11)$$

This equation is called Gross-Pitaevskii equation [12, 13, 14] and describes the time evolution of the order parameter.

1.2.3 Ground state energy

Within the formalism of the mean-field theory it is easy to obtain the ground state energy from the stationary solution of the Gross-Pitaevskii equation (1.11). To this purpose the condensate wave function should be written as $\Phi(\mathbf{r}, t) = \phi(\mathbf{r}) \exp(-i\mu t/\hbar)$, where μ is the chemical potential and the function $\phi(\mathbf{r})$ is real and normalized to the total number of particles $\int |\phi(\mathbf{r})|^2 d\mathbf{r} = N$. Then the Gross-Pitaevskii equation becomes

$$\left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) + g\phi^2(\mathbf{r}) \right) \phi(\mathbf{r}) = \mu \phi(\mathbf{r}) \quad (1.12)$$

It has the form of a nonlinear Schrödinger equation. In the absence of interactions ($g = 0$) it reduces to the usual single-particle Schrödinger equation with the Hamiltonian $-\hbar^2 \Delta / 2m + V(\mathbf{r})$.

In the uniform case, $V = 0$, $\phi(\mathbf{r})$ is a constant $\phi(\mathbf{r}) = \sqrt{n}$ and the kinetic term in (1.12) disappears. The chemical potential is given by

$$\mu = gn \quad (1.13)$$

At $T = 0$ the chemical potential is the derivative of the energy with respect to the number of particles $\mu = \partial E / \partial N$. Substitution of (1.2) into (1.13) and simple integration gives the ground state energy per particle

$$\frac{E}{N} = 4\pi(na^3)\frac{\hbar^2}{2ma^2} \quad (1.14)$$

1.2.4 Elementary excitations

In the low-temperature regime, the excited states of the system can be calculated from the “classical” frequencies of the linearized GP equation. Let us look for solutions in the form of small oscillations of the order parameter around the stationary value.

$$\Phi(\mathbf{r}, t) = e^{-i\mu t/\hbar}[\phi(\mathbf{r}) + u(\mathbf{r})e^{-i\omega t} + v^*(\mathbf{r})e^{i\omega t}] \quad (1.15)$$

By keeping terms linear in the complex functions u and v , equation (1.11) becomes

$$\begin{cases} \hbar\omega u(\mathbf{r}) &= [H_0 - \mu + 2g\phi^2(\mathbf{r})]u(\mathbf{r}) + g\phi^2(\mathbf{r})v(\mathbf{r}) \\ -\hbar\omega v(\mathbf{r}) &= [H_0 - \mu + 2g\phi^2(\mathbf{r})]v(\mathbf{r}) + g\phi^2(\mathbf{r})u(\mathbf{r}) \end{cases} \quad (1.16)$$

where $H_0 = -\hbar^2\Delta/2m + V$.

In a uniform gas, the amplitudes u and v are plane waves and the resulting dispersion law takes the Bogoliubov form

$$(\hbar\omega)^2 = \left(\frac{\hbar^2 k^2}{2m}\right) \left(\frac{\hbar^2 k^2}{2m} + 2gn\right), \quad (1.17)$$

where \mathbf{k} is the wave vector of the excitations and $n = |\phi|^2$ is the density of the gas. For large momenta the spectrum coincides with the free-particle energy $\hbar^2 k^2 / 2m$. At low momenta equation (1.17) yields the phonon dispersion $\omega = ck$, where the sound velocity c is given by the formula

$$c = \sqrt{\frac{gn}{m}} \quad (1.18)$$

1.3 Beyond mean-field: Bogoliubov theory

1.3.1 Bogoliubov Hamiltonian and elementary excitations

In the absence of the external potential $V(\mathbf{r})$, the Hamiltonian (1.1) can be conveniently expressed in momentum space

$$\hat{H} = \sum \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2} \sum \langle \mathbf{p}_1, \mathbf{p}_2 | U | \mathbf{p}'_1, \mathbf{p}'_2 \rangle \hat{a}_{\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{p}_2}^\dagger \hat{a}_{\mathbf{p}'_1} \hat{a}_{\mathbf{p}'_2} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}'_1 + \mathbf{p}'_2}, \quad (1.19)$$

where the summation is carried out over all indices that appear twice. By assuming that the relevant scattering processes involve particles at low momenta, the matrix elements in the Hamiltonian (1.19) can be replaced by their values at zero momenta, then

$$\hat{H} = \sum \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{U_0}{2V} \sum \hat{a}_{\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{p}_2}^\dagger \hat{a}_{\mathbf{p}'_1} \hat{a}_{\mathbf{p}'_2} \quad (1.20)$$

In a dilute gas almost all particles are found in the condensed state $N \approx N_0 = \hat{a}_0^\dagger \hat{a}_0$, then, as it was already discussed above (see eq. (1.7)) the operators \hat{a}_0 and \hat{a}_0^\dagger can

be treated as ordinary numbers.

The application of perturbation theory means that the last term in (1.20) should be decomposed in powers of the small quantities $\hat{a}_{\mathbf{p}}^\dagger$ and $\hat{a}_{\mathbf{p}}$, with $\mathbf{p} \neq \mathbf{0}$. The zeroth term is

$$\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 = a_0^4 \quad (1.21)$$

The first order terms are absent because they do not satisfy the law of momentum conservation. The second order terms are

$$a_0^2 \sum_{\mathbf{p} \neq \mathbf{0}} (\hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + 4\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}) \quad (1.22)$$

Here the $a_0^2 = N_0$ factor can be substituted with the total number of particles N , although in equation (1.21) it is necessary to use the more precise formula

$$a_0^2 + \sum_{\mathbf{p} \neq \mathbf{0}} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} = N \quad (1.23)$$

As a result the sum of equations (1.21) and (1.22) becomes equal to

$$N^2 + N \sum_{\mathbf{p} \neq \mathbf{0}} (\hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + 2\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}) \quad (1.24)$$

and substitution into Hamiltonian (1.20) gives

$$\hat{H} = \frac{N^2}{2V}U_0 + \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{N}{2V}U_0 \sum_{\mathbf{p} \neq 0} (\hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + 2\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}) \quad (1.25)$$

The matrix element U_0 has to be expressed in terms of the scattering length a . In the second order terms this can be done using the first Born approximation $U_0 = 4\pi\hbar^2 a/m$, although in the zeroth order term one should use the second Born approximation for collisions of two particles from the condensate

$$U_0 = \frac{4\pi\hbar^2 a}{m} \left(1 + \frac{4\pi\hbar^2 a}{V} \sum_{\mathbf{p} \neq 0} \frac{1}{p^2} \right) \quad (1.26)$$

or by introducing the speed of sound (see equation (1.18))

$$c = \sqrt{\frac{4\pi\hbar^2 a N}{m^2 V}} \quad (1.27)$$

one obtains

$$U_0 = \frac{Vmc^2}{N} \left(1 + \frac{1}{N} \sum_{\mathbf{p} \neq 0} \left(\frac{mc}{p} \right)^2 \right) \quad (1.28)$$

Substitution of this formula into (1.25) gives

$$\begin{aligned} \hat{H} = & \frac{N}{2}mc^2 \left(1 + \frac{1}{N} \sum_{\mathbf{p} \neq 0} \left(\frac{mc}{p} \right)^2 \right) + \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \\ & + \frac{mc^2}{2} \sum_{\mathbf{p} \neq 0} (\hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + 2\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}) \end{aligned} \quad (1.29)$$

In order to calculate the energy levels of the system one has to diagonalize the Hamiltonian (1.29). This can be accomplished by using the *Bogoliubov canonical transformation* of the field operators [15]. The operators $\hat{a}_{\mathbf{p}}^\dagger$ and $\hat{a}_{\mathbf{p}}$ should be expressed as a linear superposition of the quasiparticle operators $\hat{b}_{\mathbf{p}}^\dagger$ and $\hat{b}_{\mathbf{p}}$

$$\begin{cases} \hat{a}_{\mathbf{p}} &= u_p \hat{b}_{\mathbf{p}} + v_p \hat{b}_{-\mathbf{p}}^\dagger \\ \hat{a}_{\mathbf{p}}^\dagger &= u_p \hat{b}_{\mathbf{p}}^\dagger + v_p \hat{b}_{-\mathbf{p}} \end{cases} \quad (1.30)$$

which have to satisfy the same commutation rules as the operators $\hat{a}_{\mathbf{p}}^\dagger, \hat{a}_{\mathbf{p}}$ (see eq.(1.6))

$$[\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}^\dagger] = \delta_{\mathbf{p}\mathbf{p}'}, \quad [\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = 0, \quad [\hat{b}_{\mathbf{p}}^\dagger, \hat{b}_{\mathbf{p}'}^\dagger] = 0. \quad (1.31)$$

From the commutation rules (1.31) one can show that the coefficients must satisfy the condition $u_p^2 - v_p^2 = 1$. The transformation (1.30) can be rewritten as

$$\begin{cases} \hat{a}_{\mathbf{p}} &= \frac{\hat{b}_{\mathbf{p}} + L_p \hat{b}_{-\mathbf{p}}^\dagger}{\sqrt{1 - L_p^2}} \\ \hat{a}_{\mathbf{p}}^\dagger &= \frac{\hat{b}_{\mathbf{p}}^\dagger + L_p \hat{b}_{-\mathbf{p}}}{\sqrt{1 - L_p^2}} \end{cases} \quad (1.32)$$

Let us substitute (1.32) into the Hamiltonian (1.25) and set to zero the coefficient of the term proportional to $\hat{b}_{\mathbf{p}} \hat{b}_{-\mathbf{p}}$. This gives an equation for L_p

$$L_p^2 + 2 \frac{\frac{p^2}{2m} + mc^2}{mc^2} L_p + 1 = 0, \quad (1.33)$$

which has two solutions

$$L_p = \frac{1}{mc^2} \left(-\frac{p^2}{2m} - mc^2 \pm \sqrt{\left(\frac{p^2}{2m}\right)^2 + (pc)^2} \right) \quad (1.34)$$

The solution with negative sign is unphysical, because the $1 - L_p^2$ term in the square root in (1.32) becomes negative. Thus, the solution is

$$L_p = \frac{1}{mc^2} \left(E(p) - \frac{p^2}{2m} - mc^2 \right), \quad (1.35)$$

where $E(p)$ stands for

$$E(p) = \sqrt{\left(\frac{p^2}{2m}\right)^2 + (pc)^2} \quad (1.36)$$

The condition that the coefficient of the term proportional to $\hat{b}_{\mathbf{p}}^\dagger \hat{b}_{-\mathbf{p}}^\dagger$ be zero gives the same equation (1.33). Thus, if condition (1.35) is satisfied, the Hamiltonian has been diagonalized and has the form

$$\hat{H} = E_0 + \sum_{\mathbf{p}} E(p) \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}}, \quad (1.37)$$

where

$$E_0 = \frac{N}{2} mc^2 + \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[E(p) - \frac{p^2}{2m} - mc^2 \left(1 - \left(\frac{mc}{p} \right)^2 \right) \right] \quad (1.38)$$

From the Hamiltonian (1.37) and the commutation rules (1.31) one can identify $\hat{b}_{\mathbf{p}}$ and $\hat{b}_{\mathbf{p}}^\dagger$ as the creation and annihilation operators of quasiparticles with energy $E(p)$. The ground state energy is given by E_0 which is the energy of the “vacuum” of quasiparticles $\hat{H}|0\rangle = E_0|0\rangle$, where the “vacuum” state is defined as $\hat{b}_{\mathbf{p}}|0\rangle = 0$ for any value of $\mathbf{p} \neq \mathbf{0}$. The excited states are given by $|\mathbf{p}\rangle = \hat{b}_{\mathbf{p}}|0\rangle$ and have energy $E(p)$ and momentum \mathbf{p} .

It is interesting to note that the spectrum (1.36) of the elementary excitations was already obtained in (1.17) from the Gross-Pitaevskii equations by considering small oscillations of the order parameter around the stationary solution.

1.3.2 Ground state energy

In equation (1.38) the discrete summation over momenta in a volume V should be replaced by integration over $V\mathbf{dp}/(2\pi\hbar)^3$. The result is

$$\frac{E_0}{N} = \frac{mc^2}{2} \left(1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} \right) \quad (1.39)$$

The first term of this expression gives the mean-field energy and coincides with the result obtained from the Gross-Pitaevskii equation (1.14). The second term gives the correction to the ground state energy arising from the zero-point motion of the quasiparticles

$$\frac{E_0}{N} = \frac{\hbar^2}{2ma^2} \left(4\pi na^3 + \frac{512\sqrt{\pi}}{15} (na^3)^{3/2} \right) \quad (1.40)$$

The result is valid if the system is dilute, i.e. if the gas parameter is small $na^3 \ll 1$.

1.3.3 Quantum depletion of the condensate

Another interesting result that can be obtained from Bogoliubov theory is the momentum distribution of the particles. The number of particles with momentum \mathbf{p} is given by $N_{\mathbf{p}} = \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}$ or using the transformation (1.32) it is given by

$$N_{\mathbf{p}} = \frac{n_{\mathbf{p}} + L_p^2(n_{\mathbf{p}} + 1)}{1 - L_p^2}, \quad (1.41)$$

here $n_{\mathbf{p}} = \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}}$ is the number of elementary excitations, which satisfy the usual Bose distribution $n_p = (\exp\{E(p)/k_B T\} - 1)^{-1}$. At zero temperature such excitations are absent and (1.41) simplifies to

$$N_p = \frac{(mc^2)^2}{2E(p) \left[E(p) + \frac{p^2}{2m} + mc^2 \right]} \quad (1.42)$$

As $p \rightarrow 0$ the momentum distribution diverges as $N_p \rightarrow mc/2p$. The number of atoms in the condensate can be obtained by taking the difference between N and the number of non-condensed atoms.

$$N_0 = N - \sum_{\mathbf{p} \neq 0} N_p = N - \frac{V}{(2\pi\hbar)^3} \int N_p d\mathbf{p} \quad (1.43)$$

The integration can be carried out and gives the result

$$N_0 = N \left(1 - \frac{8}{3\sqrt{\pi}} (na^3)^{1/2} \right) \quad (1.44)$$

Due to interactions particles are pushed out of the condensate and a fraction

of particles with nonzero momenta is present even at zero temperature. This phenomenon is called *quantum depletion of the condensate*

Also result (1.44) is valid in the dilute regime $na^3 \ll 1$ in which the quantum depletion is small and Bogoliubov theory applies.

1.3.4 One-body density matrix

For a homogeneous system the one body density matrix is defined as the Fourier transform of the momentum distribution (1.42)

$$\rho(\mathbf{r}) = \frac{N_0}{V} + \int N_{\mathbf{p}} e^{i\mathbf{p}\mathbf{r}/\hbar} \frac{d\mathbf{p}}{(2\pi\hbar)^3}, \quad (1.45)$$

where the contribution of the condensate has been extracted from the integral. After angular integration one gets

$$\rho(r) = \frac{N_0}{V} + \rho^{(1)}(r) = \frac{N_0}{V} + \frac{1}{2\pi^2 r} \int_0^\infty N_p \sin\left(\frac{pr}{\hbar}\right) \frac{p dp}{\hbar^2} \quad (1.46)$$

At $T = 0$ the momentum distribution N_p is given by (1.42). By introducing the dimensionless variable $\xi = p/mc$, one obtains the following result for the coordinate dependent part of the one-body density matrix

$$\rho^{(1)}(r) = n \frac{4}{\pi x} \int_0^\infty \frac{\sin(\sqrt{4\pi n a^3} x \xi) d\xi}{\sqrt{4 + \xi^2} (\xi \sqrt{4 + \xi^2} + \xi^2 + 2)}, \quad (1.47)$$

where $r = ax$.

For $r = 0$, $\rho^{(1)}(0) = \frac{8}{3\sqrt{\pi}}(na^3)^{3/2}$ and the one-body density matrix coincides with the total density $\rho(0) = n$. For $r \gg r_0$ (where $r_0 = \hbar/mc = a/\sqrt{8\pi n a^3}$ is the healing

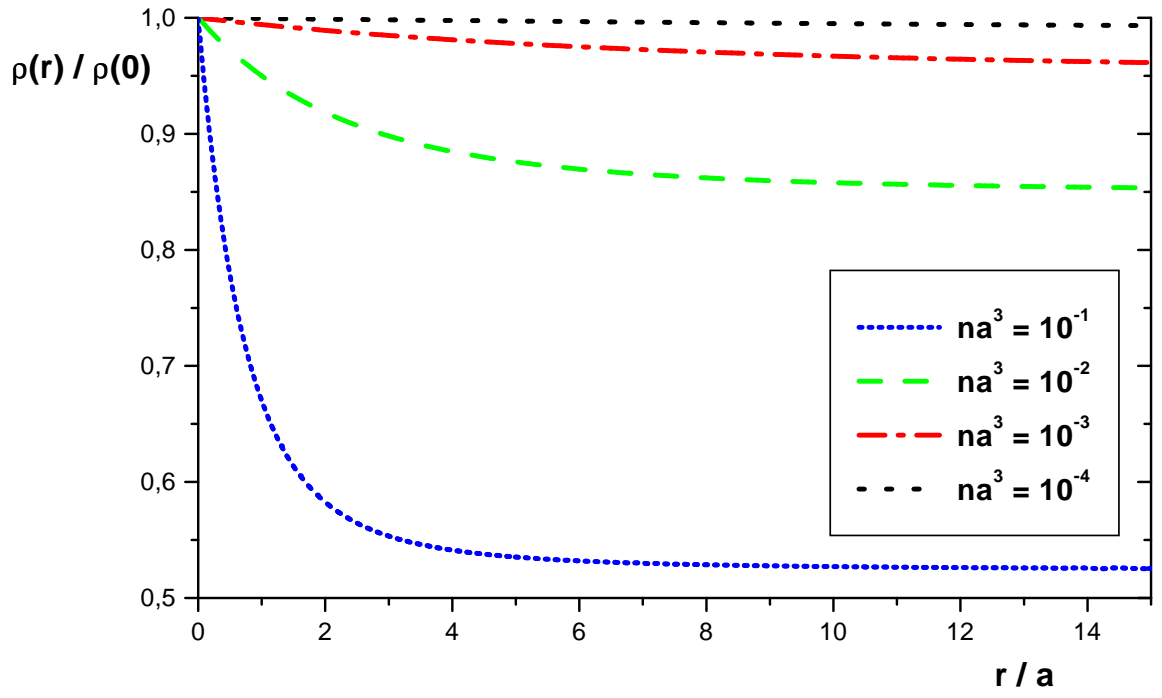


Figure 1.1: One-body density matrix

length) $\rho^{(1)}(r) = \sqrt{na}/(2\pi\sqrt{\pi}r^2)$ (see derivation and comments in Appendix B). Thus the asymptotic value of the one-body density matrix coincides with the condensate density $\lim_{r \rightarrow \infty} \rho(r) = N_0/V$.

For arbitrary values of r the integral (1.47) can be calculated numerically. Results for different values of na^3 are shown in Fig. 1.1

Chapter 2

Dilute Bose gas with disorder: perturbation expansion

2.1 Introduction

In this chapter we discuss the theory of a dilute Bose gas in the presence of disorder.

Within the Bogoliubov model we study the effects of a weak external random potential, which is modeled by a uniform random distribution of quenched impurities. We calculate the corrections to the ground state energy and to the condensate fraction due to the external random potential. We also investigate the behavior of the one-body density matrix.

The second part of this chapter is devoted to the microscopic definition of the superfluid density. By using the Bogoliubov model we study the effect of the external field on the superfluid density. This result is also obtained in a new alternative way which makes use of the Gross-Pitaevskii equation.

2.2 Bogoliubov theory in the presence of disorder

2.2.1 Random external potential

As a simple model for disorder we use the potential produced by a uniform random distribution of quenched impurities. The random external potential is then given by

$$V(\mathbf{r}) = \sum_{i=1}^{N_{imp}} v_{imp}(\mathbf{r} - \mathbf{r}_i), \quad (2.1)$$

where N_{imp} is the number of impurities present in the volume V located at the fixed positions \mathbf{r}_i , $i = \overline{1, N_{imp}}$ and $v_{imp}(\mathbf{r})$ is a two-body potential which describes the particle-impurity interaction.

This model of disorder is particularly convenient for two reasons:

- it can be easily treated analytically within the Bogoliubov theory of a dilute Bose gas
- can be easily implemented in a numerical simulation.

If the gas of impurities is dilute, as it is the case in the “weak” disorder regime which is of interest here, the particle-impurity interaction potential can be replaced by a pseudopotential

$$V(\mathbf{r}) = \sum_{i=1}^{N_{imp}} g_{imp} \delta(\mathbf{r} - \mathbf{r}_i), \quad (2.2)$$

The coupling constant g_{imp} is defined by the s -wave scattering length b of the particle-impurity collision process

$$g_{imp} = \frac{2\pi\hbar^2 b}{m}, \quad (2.3)$$

here m is the mass of the scattering particle, since the mass of the impurity is taken to be infinite (quenched impurities). In this case the particle-impurity reduced mass is twice as large as the corresponding particle-particle reduced mass. This explains the factor two difference between (1.2) and (2.3).

The important quantities which describe the statistical properties of the random external potential are the mean value

$$\overline{V}_0 = \left\langle \frac{1}{V} \int V(\mathbf{r}) \mathbf{dr} \right\rangle, \quad (2.4)$$

and the correlation function $\langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle$, where $V_{\mathbf{p}}$ denotes the Fourier component

$$V_{\mathbf{p}} = \frac{1}{V} \int e^{-i\mathbf{p}\mathbf{r}/\hbar} V(\mathbf{r}) \mathbf{dr} \quad (2.5)$$

Here $\langle \dots \rangle$ means average over disorder configurations.

For our random external potential (2.2) the correlation function can be rewritten as

$$\begin{aligned} \langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle &= \left\langle \frac{1}{V^2} \iint e^{-i\mathbf{p}(\mathbf{r}_1 - \mathbf{r}_2)/\hbar} \sum_i g_{imp} \delta(\mathbf{r}_1 - \mathbf{r}_i) \sum_j g_{imp} \delta(\mathbf{r}_2 - \mathbf{r}_j) \mathbf{dr}_1 \mathbf{dr}_2 \right\rangle = \\ &= \frac{g_{imp}^2}{V^2} \sum_i \sum_j \langle e^{-i\mathbf{p}(\mathbf{r}_1 - \mathbf{r}_i)/\hbar} \rangle \end{aligned} \quad (2.6)$$

By assuming that the impurities have a uniform distribution the mean value of

the random potential is given by

$$\overline{V}_0 = n_{imp} g_{imp} = \frac{1}{2} m c^2 \chi \left(\frac{b}{a} \right), \quad (2.7)$$

while $\langle V_{\mathbf{p}} \rangle = 0$ for $\mathbf{p} \neq \mathbf{0}$. It can be easily shown that the correlation function becomes

$$\langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle = \frac{N_{imp} g_{imp}^2}{V^2} = \frac{1}{4} \frac{(m c^2)^2}{n V} \chi \left(\frac{b}{a} \right)^2, \quad (2.8)$$

where $n_{imp} = N_{imp}/V$ is the density of impurities and $\chi = N_{imp}/N = n_{imp}/n$ is the concentration of impurities. Eq. (2.8) implies that the external potential is treated as a short correlated white noise in momentum space with amplitude proportional to g_{imp} .

The independent parameters that describe the properties of the system are the following

na^3	gas parameter
b/a	relative size of the impurity
$\chi = n^{imp}/n$	concentration of the impurities

(2.9)

2.2.2 Diagonalization of the Hamiltonian

Let us rewrite Hamiltonian (1.1) in terms of the creation and annihilation operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ in momentum representation

$$\begin{aligned}\hat{H} = & \sum \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2} \sum \langle \mathbf{p}_1, \mathbf{p}_2 | U | \mathbf{p}'_1, \mathbf{p}'_2 \rangle \hat{a}_{\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{p}_2}^\dagger \hat{a}_{\mathbf{p}'_1} \hat{a}_{\mathbf{p}'_2} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}'_1 + \mathbf{p}'_2} + \\ & + \sum \langle \mathbf{p} | V | \mathbf{p}' \rangle \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}'}\end{aligned}\quad (2.10)$$

where we have included the external potential V . We use the Bogoliubov prescription $\hat{a}_0^\dagger = \hat{a}_0 = \sqrt{N_0}$ and we consider $\hat{a}_{\mathbf{p}}, \mathbf{p} \neq \mathbf{0}$ as small perturbations. To second order in $\hat{a}_{\mathbf{p}}^\dagger$ for $\hat{a}_{\mathbf{p}}$ the external potential term can be written as

$$\sum \langle \mathbf{p} | V | \mathbf{p}' \rangle \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}'} = \sum V_{\mathbf{p}-\mathbf{p}'} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}'} \approx N_0 \overline{V}_0 + \sqrt{N_0} \sum (\hat{a}_{\mathbf{p}}^\dagger V_{\mathbf{p}} + \hat{a}_{\mathbf{p}} V_{-\mathbf{p}}), \quad (2.11)$$

The term $N_0 \overline{V}_0$ must be calculated in the second Born approximation in order to obtain an expression which is correct up to second order in the particle-impurity scattering amplitude.

$$\overline{V}_0 = \frac{mc^2}{2} \chi \left(\frac{b}{a} \right) + \frac{mc^2}{2N} \chi \left(\frac{b}{a} \right)^2 \sum_{\mathbf{p} \neq \mathbf{0}} \left(\frac{mc}{p} \right)^2 \quad (2.12)$$

The part of the Hamiltonian which is independent of the external potential can be diagonalized by the Bogoliubov transformation (1.30). The Hamiltonian takes the form

$$\begin{aligned}\hat{H} = & N \frac{mc^2}{2} \left(1 + \chi \frac{b}{a} \right) + \frac{1}{2} \sum_{\mathbf{p} \neq \mathbf{0}} \left[E(p) - \frac{p^2}{2m} - mc^2 \left\{ 1 - \left(\frac{mc}{p} \right)^2 - \chi \left(\frac{b}{a} \right)^2 \left(\frac{mc}{p} \right)^2 \right\} \right] + \\ & + \sum_{\mathbf{p} \neq \mathbf{0}} E(p) \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}} + \sqrt{N_0} \sum_{\mathbf{p} \neq \mathbf{0}} \left(\frac{\hat{b}_{\mathbf{p}} + L_p \hat{b}_{-\mathbf{p}}^\dagger}{\sqrt{1 - L_p^2}} V_{\mathbf{p}} + \frac{\hat{b}_{\mathbf{p}}^\dagger + L_p \hat{b}_{-\mathbf{p}}}{\sqrt{1 - L_p^2}} V_{-\mathbf{p}} \right)\end{aligned}\quad (2.13)$$

where E_p and L_p are defined by (1.36) and (1.35) respectively.

The linear term in the quasiparticle operators can be eliminated by means of the following transformation (analogous transformation, but for a different model of the disorder was introduced in [16])

$$\begin{cases} \hat{b}_{\mathbf{p}} &= \hat{c}_{\mathbf{p}} + Z_p V_{\mathbf{p}} \\ \hat{b}_{\mathbf{p}}^\dagger &= \hat{c}_{\mathbf{p}}^\dagger + Z_p V_{-\mathbf{p}} \end{cases} \quad (2.14)$$

with Z_p defined by

$$Z_p = -\sqrt{\frac{1+L_p}{1-L_p}} \frac{\sqrt{N_0}}{E(p)} = -\sqrt{\frac{p^2}{2mE(p)}} \frac{\sqrt{N_0}}{E(p)} \quad (2.15)$$

The transformation (2.14) does not change the commutation rules and the new quasiparticle operators $\hat{c}_{\mathbf{p}}, \hat{c}_{\mathbf{p}}^\dagger$ satisfy the usual bosonic commutation relations.

Finally, the Hamiltonian takes the form

$$\begin{aligned} \hat{H} &= N \frac{mc^2}{2} \left(1 + \chi \frac{b}{a} \right) + \sum_{\mathbf{p} \neq 0} E(p) \hat{c}_{\mathbf{p}}^\dagger \hat{c}_{\mathbf{p}} + \\ &+ \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[E(p) - \frac{p^2}{2m} - mc^2 \left\{ 1 - \left(\frac{mc}{p} \right)^2 \left(1 + \chi \left(\frac{b}{a} \right)^2 \right) \right\} - 2N_0 \frac{p^2}{2m} \frac{\langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle}{E(p)^2} \right] \end{aligned} \quad (2.16)$$

The creation and annihilation particle operators $\hat{a}_{\mathbf{p}}^\dagger, \hat{a}_{\mathbf{p}}$ are obtained from the corresponding quasiparticle operators $\hat{c}_{\mathbf{p}}^\dagger, \hat{c}_{\mathbf{p}}$ in the following way

$$\begin{cases} \hat{a}_{\mathbf{p}} &= \frac{\hat{c}_{\mathbf{p}} + L_p \hat{c}_{-\mathbf{p}}^\dagger}{\sqrt{1-L_p^2}} - \sqrt{N_0} \frac{1+L_p}{1-L_p} \frac{V_{\mathbf{p}}}{E_p} = \frac{\hat{c}_{\mathbf{p}} + L_p \hat{c}_{-\mathbf{p}}^\dagger}{\sqrt{1-L_p^2}} - \sqrt{N_0} \frac{p^2}{2m} \frac{V_{\mathbf{p}}}{E^2(p)} \\ \hat{a}_{\mathbf{p}}^\dagger &= \frac{\hat{c}_{\mathbf{p}}^\dagger + L_p \hat{c}_{-\mathbf{p}}}{\sqrt{1-L_p^2}} - \sqrt{N_0} \frac{1+L_p}{1-L_p} \frac{V_{-\mathbf{p}}}{E_p} = \frac{\hat{c}_{\mathbf{p}}^\dagger + L_p \hat{c}_{-\mathbf{p}}}{\sqrt{1-L_p^2}} - \sqrt{N_0} \frac{p^2}{2m} \frac{V_{-\mathbf{p}}}{E^2(p)} \end{cases} \quad (2.17)$$

2.2.3 Ground state energy

By inserting the results (2.7) and (2.8) for \overline{V}_0 and $\langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle$ respectively into the Hamiltonian (2.16) and after integration one gets the following result for the ground state energy

$$\frac{E_0}{N} = \frac{\hbar^2}{2ma^2} \left\{ 4\pi na^3 \left(1 + \chi \frac{b}{a} \right) + (na^3)^{3/2} \left(\frac{512\sqrt{\pi}}{15} + 16\pi^{3/2} \chi \left(\frac{b}{a} \right)^2 \right) \right\} \quad (2.18)$$

The first term in the above equation simply gives the mean field energy (see eq.(1.14)) with the correction due to the presence of the random external potential. This becomes clearer if we rewrite this term in terms of the coupling constant $E_{MF} = 1/2(gn + g_{imp}n_{imp})$. The beyond mean-field correction to the ground state energy is given by

$$\frac{E_0}{N} - \frac{E_{MF}}{N} = \frac{\hbar^2}{2ma^2} (na^3)^{3/2} \left(\frac{512\sqrt{\pi}}{15} + 16\pi^{3/2} \chi \left(\frac{b}{a} \right)^2 \right) \quad (2.19)$$

The correction due to disorder in the above result is proportional to

$$R = \chi \left(\frac{b}{a} \right)^2, \quad (2.20)$$

which as we will see represents an important parameter to describe the effect of disorder.

2.2.4 Quantum depletion of the condensate

It is easy to obtain the particle momentum distribution $\langle N_{\mathbf{p}} \rangle = \langle \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} \rangle$ from the operator transformation (2.17).

$$\langle N_{\mathbf{p}} \rangle = \frac{\langle n_{\mathbf{p}} \rangle + L_p^2(\langle n_{\mathbf{p}} \rangle + 1)}{1 - L_p^2} + \left(\frac{p^2}{2m} \right)^2 \frac{\langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle}{E^4(p)} N_0, \quad (2.21)$$

where $\langle n_{\mathbf{p}} \rangle$ is the number of excitations with momentum \mathbf{p} . At zero temperature such excitations are absent and the distribution (2.21) takes the form

$$\begin{aligned} \langle N_{\mathbf{p}} \rangle &= \frac{L_p^2}{1 - L_p^2} + \left(\frac{p^2}{2m} \right)^2 \frac{\langle V_{\mathbf{p}} V_{-\mathbf{p}} \rangle}{E^4(p)} = \\ &= \frac{(mc^2)^2}{2E(p)(E(p) + \frac{p^2}{2m} + mc^2)} + \frac{\chi \left(\frac{b}{a} \right)^2}{\left(4 + \left(\frac{p}{mc} \right)^2 \right)^2} \end{aligned} \quad (2.22)$$

The first term of the above result corresponds to the momentum distribution in the absence of disorder. The second term gives the contribution due to disorder. The presence of disorder induces an extra quantum depletion of the condensate arising from the particle-impurity interaction. By integrating over momentum one obtains the following result for the condensate fraction

$$\frac{N_0}{N} = 1 - \frac{8}{3\sqrt{\pi}}(na^3)^{1/2} - \frac{\sqrt{\pi}}{2}(na^3)^{1/2}\chi \left(\frac{b}{a} \right)^2 \quad (2.23)$$

It is interesting to note, that the effect of disorder again is described by the combination of parameters $R = \chi(b/a)^2$, as it was found for the energy (2.18).

2.2.5 One body density matrix

The one body density matrix is given by the Fourier transform of the momentum distribution (see (1.45)). There are three contributions to the one-body density matrix coming from condensate, particle-particle interaction effects and particle-impurity interaction effects:

$$\rho(r) = \frac{N_0}{V} + \rho^{(1)}(r) + \rho^{(2)}(r) \quad (2.24)$$

The result for $\rho^{(1)}(r)$ has been given in (1.47). Here we calculate the contribution due to disorder

$$\rho^{(2)}(r) = \frac{2\chi \left(\frac{b}{a}\right)^2}{\pi V x} \int_0^\infty \frac{\sin(\sqrt{4\pi n a^3 x} \xi)}{(4 + \xi^2)^2} \xi d\xi = \frac{\sqrt{\pi}}{2} \sqrt{n a^3} \chi \left(\frac{b}{a}\right)^2 \exp\left(-\frac{r}{\sqrt{2} r_0}\right) n, \quad (2.25)$$

where $r_0 = a/\sqrt{8\pi n a^3}$ is the healing length.

Notice that at $r = 0$ the value of the integral equals to the density of particles which are scattered out of the condensate due to the presence of the external field.

2.3 Superfluid density

2.3.1 Connection between ρ_s/ρ and the transverse current-current response function

One of the striking properties of superfluids is the ability to flow without friction. This fact allows us to define the normal fluid density ρ_n as the fraction of liquid which is carried along by the walls if they are set in motion. For example [17, 18], consider the liquid inside a long tube (see. Fig 2.1), which was at rest at time $t = -\infty$ and was

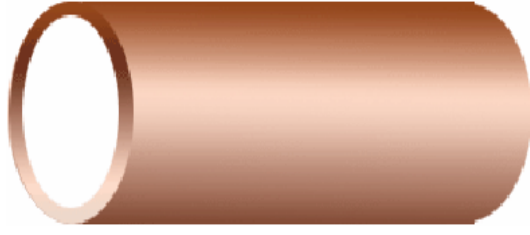


Figure 2.1: Long tube filled with superfluid

then adiabatically accelerated up to time $t = 0$ (for instance with the exponential law $v(t) = v \exp(\varepsilon t)$ with infinitesimal $\varepsilon > 0$). The normal component ρ_n can be defined through the momentum density $\langle \vec{j} \rangle$ at $t = 0$

$$\langle \vec{j} \rangle = \rho_n \vec{v} \quad (2.26)$$

and the superfluid density as the difference between the total density ρ and ρ_n

$$\rho_s = \rho - \rho_n \quad (2.27)$$

The effect of the perturbation caused by the moving walls is given by the energy

$$V_{walls} = - \int \vec{j}(x) \vec{v}(x, t) d^3x, \quad (2.28)$$

where $\vec{j}(x)$ is the momentum density and $\vec{v}(x, t)$ is the external velocity field. The linear response is given by the Kubo formula

$$\langle j_i(x, t) \rangle = \int_{-\infty}^{\infty} ds \int d^3y \chi_{ij}(x, t; y, s) v_j(y, s), \quad (2.29)$$

where

$$\chi_{ij}(x, t; y, s) = i\theta(t - s) \langle [j_i(x, t), j_j(y, s)] \rangle \quad (2.30)$$

For uniform systems the response function χ_{ij} depends only on the difference of its arguments $\chi_{ij} = \chi_{ij}(x - y, t - s)$. The *static susceptibility* is defined as

$$\chi_{ij}(x) = \int_{-\infty}^0 \chi_{ij}(x, t) e^{\varepsilon t} dt \quad (2.31)$$

or in terms of Fourier components

$$\chi_{ij}(k) = \int_{-\infty}^{\infty} \frac{\chi_{ij}(k, \omega)}{\omega + i\varepsilon} \frac{d\omega}{2\pi} \quad (2.32)$$

At time $t = 0$ the linear response function satisfies the equation

$$\langle j_i(k) \rangle = \chi_{ij}(k) v_j(k), \quad i, j = \{x, y, z\} \quad (2.33)$$

Since $\chi_{ij}(k)$ is a second rank tensor, it can be decomposed into the sum of longitudinal and transverse components

$$\chi_{ij}(k) = \frac{k_i k_j}{k^2} \chi_L(k) + \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \chi_T(k), \quad (2.34)$$

Let us consider first the transverse response. Due to the rotational invariance of $\chi_T(k)$ it is enough to examine the response in an arbitrary direction, for example

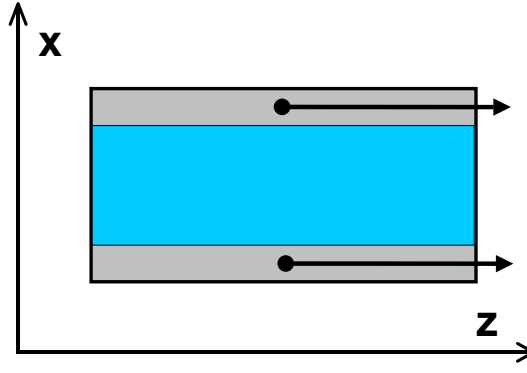


Figure 2.2: Illustration of the transverse response. Only the normal component is dragged in z direction

χ_{zz} , that is the momentum response $j_z(\mathbf{k})$ due to an imposed velocity field in the z direction $v_z(\mathbf{k})$.

Suppose first that the velocity field is created by dragging the walls of an indefinitely long pipe (see Fig. 2.2) and the cross section of the pipe tends to infinity. This arrangement corresponds to the limiting procedure $k_z \rightarrow 0$, followed by $k_x \rightarrow 0$, $k_y \rightarrow 0$. Then, the part of the system responding to the shear force is defined as the normal fluid. Carrying out the limiting procedure $k^2 = k_x^2 + k_y^2 + k_z^2 \rightarrow 0$ gives

$$\rho_n = \lim_{\substack{k_x \rightarrow 0 \\ k_y \rightarrow 0}} \lim_{k_z \rightarrow 0} \chi_{ij}(k) = \lim_{k \rightarrow 0} \chi_T(k) \quad (2.35)$$

Next suppose that the pipe of infinite radius is constrained by two plates, normal to the z axis, with separation between the plates approaching infinity, as illustrated in Fig. 2.3. In this case the entire fluid $\rho = \rho_s + \rho_n$ responds to the external probe. This arrangement corresponds to the limiting procedure $k_x \rightarrow 0$, $k_y \rightarrow 0$, followed by $k_z \rightarrow 0$. The result of the limiting procedure is

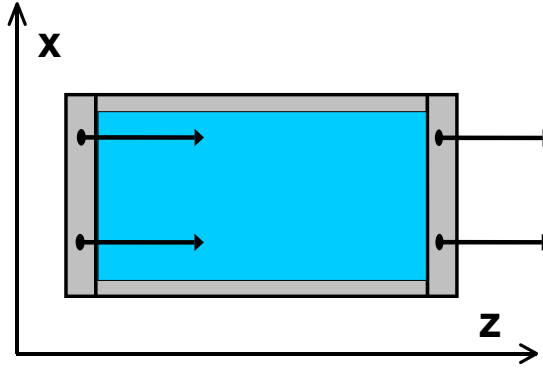


Figure 2.3: Illustration to the longitudinal response. Both superfluid and normal components are pushed in the z direction

$$\rho = \lim_{k_z \rightarrow 0} \lim_{\substack{k_x \rightarrow 0 \\ k_y \rightarrow 0}} \chi_{ij}(k) = \lim_{k \rightarrow 0} \chi_L(k) \quad (2.36)$$

2.3.2 Superfluid fraction ρ_s/ρ in the presence of disorder

Let us apply the theory developed in the previous section to a dilute Bose system. As we will see, the system without disorder is fully superfluid at zero temperature while the presence of impurities create a depletion of the superfluid density.

According to (2.34) and (2.35) the normal component is given by the limit of the transverse current-current response function. Let us consider, for example, $\chi_T = \chi_z$, i.e. z response and in the z direction (see Fig. 2.2). First one has to take the limit $k_z \rightarrow 0$ and after $k_x \rightarrow 0$ and $k_y \rightarrow 0$. This can be accomplished by considering $\mathbf{k} = (k, 0, 0)$ and letting k decrease toward zero.

The k -component of the current operator \hat{j} in second quantization is given by the formula

$$\hat{j}_{\mathbf{k}} = \frac{\hbar}{\sqrt{V}} \sum_{\mathbf{q}} \left(\mathbf{q} + \frac{\mathbf{k}}{2} \right) \hat{a}_{\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{q}+\mathbf{k}}, \quad (2.37)$$

where in the absence of disorder the particle creation and annihilation operators can be expressed in terms of quasiparticle operators by means of the Bogoliubov transformation (1.32). Once the current (2.37) is calculated, the transverse response function can be obtained by averaging the commutator

$$\chi_T(\mathbf{k}, t) = -i\Theta(t) \langle [j_{\mathbf{k}}^z(t), j_{-\mathbf{k}}^z(0)] \rangle \quad (2.38)$$

By taking the Fourier transform

$$\chi_T(\mathbf{k}, \omega) = \int_{-\infty}^{+\infty} \exp(i\omega t) \chi_T(\mathbf{k}, t) dt \quad (2.39)$$

the limiting procedure

$$\rho_n = \lim_{k \rightarrow 0} \lim_{\omega \rightarrow 0} \chi_T(k, \omega) \quad (2.40)$$

yields the density of the normal fluid.

It is easy to check that in the absence of disorder $\chi_T(\mathbf{k}, \omega)$ goes to zero as $\mathbf{k} \rightarrow \mathbf{0}$ and $\omega \rightarrow 0$ that the commutator (2.38) of χ_{zz} goes to zero in the limit $k \rightarrow 0$. This corresponds to the fact that a homogeneous dilute Bose gas is completely superfluid at $T = 0$.

A useful check consists in the calculation of the longitudinal response (see Fig. 2.3).

This means taking first the limit $k_x \rightarrow 0, k_y \rightarrow 0$ in $\chi_{zz}(\mathbf{k})$. We consider $\mathbf{k} = (0, 0, k)$ and then let $k \rightarrow 0$. It is easy to calculate χ_{zz} in Bogloliubov approximation.

For the z component of the current operator one has

$$\hat{j}_{\mathbf{k}}^z = \frac{\hbar \mathbf{k} \sqrt{N_0}}{\sqrt{V}} \frac{(\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger)}{2} + \frac{\hbar}{\sqrt{V}} \sum_{\mathbf{q} \neq 0} \left(\mathbf{q} + \frac{\mathbf{k}}{2} \right) \hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}+\mathbf{k}}, \approx \frac{\hbar \mathbf{k} \sqrt{N_0}}{\sqrt{V}} \frac{(\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger)}{2} \quad (2.41)$$

Within this level of accuracy the limit (2.36) of the longitudinal component is given by

$$\lim_{\mathbf{k} \rightarrow 0} \lim_{\omega \rightarrow 0} \chi_L(\mathbf{k}, \omega) = n_0 m \approx nm \quad (2.42)$$

Let us now study the system in the presence of the random external potential. Starting from the transformation (2.17) between the particles operators $\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}}^\dagger$ and the corresponding quasiparticle operators $\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}}^\dagger$ one can write the contribution to the current proportional to the external potential (there is no need to consider the contribution independent of the external potential, because as calculated before it is equal to zero).

$$\hat{j}_0^z(t) = \sum_{\mathbf{q}} \frac{\hbar q_z Z_q}{\sqrt{V}} \sqrt{\frac{1 - L_q}{1 + L_q}} (\hat{c}_{\mathbf{q}}^\dagger V_{-\mathbf{q}} - \hat{c}_{\mathbf{q}} V_{\mathbf{q}}) + \dots \quad (2.43)$$

Notice that in order to make calculations simpler we take $k = 0$ from the very begging. Result (2.35) is independent of the order of the two limits.

The response function is then given by

$$\chi_T(0, t) = -i\Theta(t)\frac{1}{V}\sum_{\mathbf{q}}\hbar^2q_x^2|Z_q|^2\langle V_{\mathbf{q}}V_{-\mathbf{q}}\rangle\frac{1-L_q}{1+L_q}(e^{-i\omega_{\mathbf{q}}t} - e^{i\omega_{\mathbf{q}}t}) \quad (2.44)$$

its Fourier transformation being equal to

$$\chi_T(0, w) = \frac{1}{V}\sum_{\mathbf{q}}\hbar^2q_x^2|Z_q|^2\langle V_{\mathbf{q}}V_{-\mathbf{q}}\rangle\frac{1-L_q}{1+L_q}\left(\frac{1}{\omega-\omega_q} - \frac{1}{\omega+\omega_q}\right), \quad (2.45)$$

and, finally, setting $\omega = 0$ one obtains

$$\rho_n = \chi_T(0, 0) = \frac{4m\hbar}{3V}\sum_q q_x^2|Z_q|^2\langle V_qV_{-q}\rangle = \frac{2\sqrt{\pi}}{3}(na^3)^{1/2}\chi\left(\frac{b}{a}\right)^2 nm \quad (2.46)$$

This result gives the depletion of the superfluid density due to the presence of impurities.

2.3.3 calculation of the superfluid fraction from GPE

In this section the superfluid fraction ρ_s/ρ will be obtained directly from Gross-Pitaevskii equation in a perturbative way. This derivation is new and the result coincides with the one obtained from the Bogoliubov model presented in the previous section.

The Gross-Pitaevskii equation (1.11) for the condensate wavefunction in the absence of external field takes the form

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m}\Delta + g|\Psi(\mathbf{r}, t)|^2\right)\Psi(\mathbf{r}, t) \quad (2.47)$$

Let us add a moving impurity that creates an external field $V_{ext}(\mathbf{r}, t) = g_{imp}\delta(\mathbf{r} - \mathbf{V}t)$ and let us treat it as a perturbation to the solution $\Psi_0(\mathbf{r}, t)$ of the equation (2.47), i.e.

$$\Psi(\mathbf{r}, t) = [\Psi_0(\mathbf{r}) + \delta\Psi(\mathbf{r}, t)] \exp\left(-i\frac{\mu t}{\hbar}\right), \quad (2.48)$$

Then, substitution of (2.48) into (2.47) gives

$$i\hbar \frac{\partial}{\partial t} \delta\Psi = \left(-\frac{\hbar^2}{2m} \Delta - \mu\right) \delta\Psi + 2g|\Psi_0|^2 \delta\Psi + g\Psi_0^2 \delta\Psi^* + g_{imp}\delta(\mathbf{r} - \mathbf{V}t)\Psi_0 \quad (2.49)$$

The perturbation follows the moving impurity, so $\delta\Psi$ is a function of $\mathbf{r} - \mathbf{V}t$.

Let us introduce the new variable $\mathbf{r}' = \mathbf{r} - \mathbf{V}t$. It means that the coordinate derivative can be related to time derivative

$$\frac{\partial}{\partial t} \delta\Psi(\mathbf{r} - \mathbf{V}t) = -\mathbf{V} \nabla \delta\Psi(\mathbf{r} - \mathbf{V}t), \quad (2.50)$$

$$\Delta \mathbf{r}' = \Delta \mathbf{r} \quad (2.51)$$

and instead of (2.49) one has

$$\left(i\hbar \mathbf{V} \nabla - \frac{\hbar^2}{2m} \Delta - \mu + 2g|\Psi_0|^2\right) \delta\Psi + g\Psi_0(\mathbf{r})^2 \delta\Psi^* + g_{imp}\delta(\mathbf{r})\Psi_0 = 0, \quad (2.52)$$

(from now on, the subscript over \mathbf{r} will be dropped)

Taking the Fourier transform of this equation and treating Ψ_0 as a real constant (i.e. the solution for the uniform case $g\Psi_0^2 = \mu$) one obtains

$$\left(-\hbar \mathbf{k} \mathbf{V} + \frac{\hbar^2 k^2}{2m} - \mu + 2\mu\right) \delta \Psi_k + \mu \delta(\Psi_{-k})^* + g_{imp} \Psi_0 = 0, \quad (2.53)$$

where we used the property of Fourier components $\delta(\Psi^*)_k = \delta(\Psi_{-k})^*$.

The substitution of $(-\mathbf{k})$ in the equation complex conjugate of (2.53) gives

$$\left(\hbar \mathbf{k} \mathbf{V} + \frac{\hbar^2 k^2}{2m} - \mu + 2\mu\right) (\delta \Psi_{-k})^* + \mu \delta \Psi_k + g_{imp} \Psi_0 = 0 \quad (2.54)$$

The solution for the system of linear equations (2.53 - 2.54) is given by

$$\delta \Psi_k = -\frac{g_{imp} \left(\hbar \mathbf{k} \mathbf{V} + \frac{\hbar^2 k^2}{2m}\right) \Psi_0}{\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu\right) - (\hbar \mathbf{k} \mathbf{V})^2} \quad (2.55)$$

The energy $E' = E - \mu N$ has the minimum at fixed μ for the ground state function Ψ_0 . It means that E' does not have terms linear in $\delta \Psi_k$ and $\delta \Psi_k^*$, so $E' = E^{(0)} + E^{(2)} + g_{imp}(\Psi_0^* \delta \Psi(0) + \Psi_0 \delta \Psi^*(0))$. Here the last term comes from the linear expansion of the energy $\int |\Psi(\mathbf{r})|^2 g_{imp} \delta(\mathbf{r}) d\mathbf{r}$. The term $E^{(2)}$ being quadratic in $\delta \Psi_k$ and $\delta \Psi_k^*$ satisfies the Euler identity:

$$2E^{(2)} = \int \left[\delta \Psi(\mathbf{r}) \frac{\delta E^{(2)}}{\delta(\delta \Psi(\mathbf{r}))} + \delta \Psi^*(\mathbf{r}) \frac{\delta E^{(2)}}{\delta(\delta \Psi^*(\mathbf{r}))} \right] d\mathbf{r} \quad (2.56)$$

which using the variational equation

$$i\hbar \frac{\partial \delta(\delta \Psi)}{\partial t} = \frac{\delta E^{(2)}}{\delta(\delta \Psi^*)} + g_{imp} \Psi_0 \delta(\mathbf{r}) \quad (2.57)$$

can be rewritten as

$$E^{(2)} = E_1^{(2)} + E_2^{(2)} = \frac{i\hbar}{2} \int \left[\delta\Psi^*(\mathbf{r}) \frac{\partial \delta\Psi(\mathbf{r})}{\partial t} - \frac{\partial \delta\Psi^*(\mathbf{r})}{\partial t} \delta\Psi(\mathbf{r}) \right] d\mathbf{r} - \frac{g_{imp}}{2} (\Psi_0^* \delta\Psi(0) + \Psi_0 \delta\Psi^*(0)) \quad (2.58)$$

To start with, let us Fourier transform the first term. Exchanging time derivatives with gradients by the rule (2.50) one obtains

$$E_1^{(2)} = \int \hbar \mathbf{k} \mathbf{V} |\delta\Psi_k|^2 \frac{d\mathbf{k}}{(2\pi)^3} \quad (2.59)$$

The terms of interest are the ones that are quadratic in the velocity \mathbf{V} . It means that the term $(\hbar \mathbf{k} \mathbf{V})^2$ in the denominator of (2.55) can be neglected and $|\delta\Psi_k|^2$ turns out to be

$$|\delta\Psi_k|^2 = \frac{g_{imp}^2 |\Psi_0|^2 \left[\left(\frac{\hbar^2 k^2}{2m} \right)^2 + 2 \frac{\hbar^2 k^2}{2m} \hbar \mathbf{k} \mathbf{V} \right]}{\left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu \right) \right]^2} \quad (2.60)$$

The energy does not have terms linear in \mathbf{V} , because all terms independent of \mathbf{V} in (2.60) are even in \mathbf{k} , so multiplied by \mathbf{k} and integrated over momentum space they provide zero contribution to the energy. The only term that is left is the following

$$E_1^{(2)} = 2g_{imp}^2 |\Psi_0|^2 \int \frac{(\hbar \mathbf{k} \mathbf{V})^2}{\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu \right)^2} \frac{d\mathbf{k}}{(2\pi)^3} \quad (2.61)$$

For the calculation of $\delta\Psi(0)$ one should consider $\delta\Psi_k$ taking into account that $\hbar \mathbf{k} \mathbf{V} \ll \mu$ and then integrate it over momentum space

$$\begin{aligned} \delta\Psi_k \approx & \frac{(\hbar\mathbf{k}\mathbf{V})^2}{\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu \right)^2} g_{imp} \Psi_0 - \\ & - \left\{ \frac{\hbar\mathbf{k}\mathbf{V} \left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu \right) \right] + (\hbar\mathbf{k}\mathbf{V})^3}{\left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu \right) \right]^2} + \frac{1}{\frac{\hbar^2 k^2}{2m} + 2\mu} \right\} g_{imp} \Psi_0 \end{aligned} \quad (2.62)$$

The integral of the second term over momentum space is equal to zero. The third term is diverging and needs the renormalization of g_{imp} (as discussed in sections 1.3.1 and 2.2.2) in order to be calculated correctly. However, its correction does not depend on \mathbf{V} and will be omitted.

The energy is defined by the following integral

$$(2.63)$$

$$nonumber \delta E = E_1^{(2)} + E_2^{(2)} + g_{imp}(\Psi_0^* \delta\Psi(0) + \Psi_0 \delta\Psi^*(0)) = \quad (2.64)$$

$$= \left(2g_{imp}^2 |\Psi_0|^2 - \left(g_{imp} - \frac{g_{imp}}{2} \right) (\Psi_0^* \Psi_0 + \Psi_0 \Psi_0^*) \right) \int \frac{(\hbar\mathbf{k}\mathbf{V})^2 d\mathbf{k}}{\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\mu \right)^2} \frac{d\mathbf{k}}{(2\pi)^3} \quad (2.65)$$

In the integral $(\mathbf{k}\mathbf{V})^2 d\mathbf{k}$ can be replaced by $1/3 k^2 V^2 4\pi k^2 dk$ due to the equivalence of different directions. Then the integral can be easily calculated if one recall the following integral identity

$$\int \frac{x^2 dx}{(x^2 + a^2)^2} = -\frac{x}{2(x^2 + a^2)^2} + \frac{1}{2a} \operatorname{atan} \frac{x}{a} \quad (2.66)$$

The result is the following

$$\delta E = \frac{m^{5/2} g_{imp}^2 |\Psi_0|^2 V^2}{3\pi \hbar^3 \sqrt{\mu}} \frac{1}{2}, \quad (2.67)$$

where

$$g = \frac{4\pi\hbar^2 a}{m}, \quad g_{imp} = \frac{2\pi\hbar^2 b}{m}, \quad |\Psi_0|^2 = n$$

The term in front of $V^2/2$ in (2.67) can be interpreted as an effective mass m^* of the particles which follow the external perturbation, i.e. the normal (and not superfluid) component of the fluid. Then normal fraction can then be easily obtained which, as anticipated, coincides with result (2.46).

$$\frac{\rho_n}{\rho} = \frac{m^*}{m} \chi = \frac{2\sqrt{\pi}}{3} (na^3)^{1/2} \chi \left(\frac{b}{a}\right)^2 \quad (2.68)$$

Let us compare the results for the superfluid density (2.68) and the condensate fraction (2.23). It is interesting to note that in both formulae the effect of disorder enters as $\sqrt{na^3}R$, where $R = \chi(b/a)^2$ is the universal scaling parameter which already entered the result (2.18) for the energy. This means that systems with different disorder concentration χ and size of the impurities b/a , but same R experience the same effect due to disorder.

Another interesting result is that disorder is more efficient (by a factor $4/3$) in depleting the superfluid density than the condensate. Taking into account that even pure systems ($R = 0$) exhibit a nonzero quantum depletion due to particle interactions, one infers that at the critical amount of disorder $R_c = 16/\pi \approx 5.1$ the depletion of the superfluid density becomes larger than the depletion of the condensate fraction.

Huang and Meng [16], who first derived results (2.23) and (2.46) even if for a different model of disorder, have used them at $T = 0$ to predict two distinct transitions as a function of the amount of disorder : first a superfluid-insulator transition where $\rho_s = 0$ followed by a Bose-Einstein transition where $N_0 = 0$. These authors also argue

that the intermediate phase corresponding to $\rho_s = 0$ and $N_0 \neq 0$ should be identified with a Bose-glass phase. However, in [19] it is stressed that results (2.23) and (2.46) are valid in the weak disorder regime and cannot be applied if the depletion due to disorder is large.

The range of validity of results (2.23) and (2.68) will be investigated in detail in section 4.4.2 using Monte Carlo techniques.

Chapter 3

Quantum Monte Carlo Method

3.1 Diffusion Monte Carlo

3.1.1 Introduction

Monte Carlo methods are very powerful tools for the investigation of quantum many body systems (for a review see, for example, [20]).

The simplest of the quantum Monte-Carlo methods is the *variational* method (VMC). The idea of this method is to use an approximate wavefunction ψ_T for the system (trial wavefunction) and then to sample the probability distribution $p(r) = |\psi(r)|^2$ and calculate averages of physical quantities over this distribution. The average of the local energy $E_L = \psi_T^{-1} H \psi_T$ gives an upper bound to the ground-state energy. In this method one must make a good guess for the trial wavefunction, and there is no regular way for doing it and further improving it. In VMC the closer is the trial wavefunction to the stationary eigenfunction the smaller is the energy variance $\langle H^2 \rangle - \langle H \rangle^2$. In usual applications the trial wavefunction depends on the particle coordinates and on some external parameters $\psi_T = \psi_T(r_1, \dots, r_N, a, b, \dots)$. By minimizing the variational energy with respect to the external parameters one can optimize the wavefunction within the given class of wavefunctions considered.

The Diffusion Monte Carlo method (DMC) can be successfully applied to the investigation of boson systems at low temperatures. It is based on solving the Schrödinger equation in imaginary time and allows us to calculate the exact (in statistical sense) value of the ground state energy. The DMC method will be extensively discussed in the next sections.

The Path Integral Monte Carlo (PIMC) is based on carrying out discretized Feynman integral in the imaginary time which allows to calculate the density matrix of the system. The main advantage of this method is that it works at finite temperatures and one has access to the study of thermodynamic properties such as the critical behavior in the proximity of a phase transition ([21], [22]).

In this study we use DMC method because we are interested in the ground state properties of the system.

3.1.2 Schrödinger equation

The wavefunction of the system satisfies the Schrödinger equation

$$i\hbar \frac{\partial}{\partial \tau} \varphi(\mathbf{R}, \tau) = \hat{H} \varphi(\mathbf{R}, \tau), \quad (3.1)$$

where $\mathbf{R} = (\vec{r}_1, \vec{r}_2, \dots)$ denotes the particle coordinates. This equation can be rewritten in imaginary time $t = i\tau/\hbar$.

$$-\frac{\partial}{\partial t} \varphi(\mathbf{R}, t) = (\hat{H} - E) \varphi(\mathbf{R}, t), \quad (3.2)$$

where E is an energy shift whose meaning will become clearer later.

The formal solution of this equation is

$$\psi(\mathbf{R}, t) = e^{-(\hat{H}-E)t} \psi(\mathbf{R}, 0) \quad (3.3)$$

This solution can be expanded in eigenstate functions of the Hamiltonian $\hat{H}\phi_n = E_n\phi_n$, $E_0 < E_1 < \dots$

$$\psi(\mathbf{R}, t) = \sum_n c_n \phi_n(\mathbf{R}, t) = \sum_n c_n \phi_n(\mathbf{R}, 0) e^{-(E_n-E)t} \quad (3.4)$$

The amplitudes of the components change with time, either increasing or decreasing depending on the sign of $(E_n - E)$. At large times the term that corresponds to the projection on the ground state dominates the sum. In other words all excited states decay exponentially fast and only contribution from ground state survives

$$\psi(\mathbf{R}, t) \rightarrow c_0 \phi_0(\mathbf{R}, 0) e^{-(E_0-E)t} \quad \text{if } t \rightarrow \infty \quad (3.5)$$

In the long time limit the wavefunction remains finite only when E is equal to E_0 . This provides a method to obtain the ground state energy by adjusting the parameter E in a way that the norm of $\psi(\mathbf{R}, t)$ is constant.

Let us consider system of N particles, introducing the Hamiltonian through a pair-wise potential

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1} \Delta_i + \sum_{i<j}^N V(|\vec{r}_i - \vec{r}_j|), \quad (3.6)$$

and the Schrödinger equation reads

$$-\frac{\partial}{\partial t}\psi(\mathbf{R},t) = -D \sum_{i=1}^N \Delta_i \psi(\mathbf{R},t) + V(\mathbf{R})\psi(\mathbf{R},t) - E\psi(\mathbf{R},t), \quad (3.7)$$

where the following notation is used: $D = \hbar^2/2m$ and $V(\mathbf{R}) = \sum_{i<j} V(|\vec{r}_i - \vec{r}_j|)$. In principle, any external field which is independent of the particle momenta and is a function only of the particle coordinates can be included into $V(\mathbf{R})$ without any harm to the reasoning.

Better efficiency is achieved if the importance sampling is used. In the DMC method this means that one has to solve the Schrödinger equation for the modified wavefunction ¹

$$f(\mathbf{R},t) = \psi_T(\mathbf{R},t)\psi(\mathbf{R},t) \quad (3.8)$$

Here $\psi_T(\mathbf{R},t)$ is the trial wavefunction which approximates the true wavefunction $\psi(\mathbf{R},t)$ of the system. The distribution function f satisfies the following equation

$$-\frac{\partial}{\partial t}f(\mathbf{R},t) = -D \sum_{i=1}^N \Delta_i f(\mathbf{R},t) + D\vec{\nabla}(\vec{F}f(\mathbf{R},t)) + (E_L(\mathbf{R}) - E)f(\mathbf{R},t), \quad (3.9)$$

here E_L denotes the *local energy* which is the average of the Hamiltonian with respect to trial wavefunction

$$E_L(\mathbf{R}) = \frac{\psi_T^*(\mathbf{R})\hat{H}\psi_T(\mathbf{R})}{\psi_T^*(\mathbf{R})\psi_T(\mathbf{R})} \quad (3.10)$$

¹One of the reasons for using the product of wavefunctions as the probability distribution instead of sampling ψ is that the average over the latter is ill defined $\langle A \rangle = \int A\psi dR / \int \psi dR$, on the contrary the average over the product of wavefunctions has the meaning of the mixed estimator $\langle A \rangle = \int \psi_T A \psi dR / \int \psi_T \psi dR$

and \vec{F} is the *drift force* which is proportional to the gradient of the trial wave-function and consequently always points in the direction where ψ_T increases

$$\vec{F} = \frac{2}{\psi_T(\mathbf{R})} \vec{\nabla} \psi_T(\mathbf{R}) \quad (3.11)$$

3.1.3 Green's function

The formal solution of the Schrödinger equation written in coordinate space is given by

$$\langle \mathbf{R} | f(t) \rangle = \sum_{\mathbf{R}'} \langle \mathbf{R} | e^{-(\hat{H}-E)t} | \mathbf{R}' \rangle \langle \mathbf{R}' | f(0) \rangle, \quad (3.12)$$

or, expressed in terms of the Green's function $G(\mathbf{R}, \mathbf{R}', t) = \langle \mathbf{R} | e^{-(\hat{H}-E)t} | \mathbf{R}' \rangle$, the above equation reads

$$f(\mathbf{R}, t) = \int G(\mathbf{R}, \mathbf{R}', t) f(\mathbf{R}', 0) d\mathbf{R}' \quad (3.13)$$

In other words, the differential Schrödinger equation (3.3) corresponds to the integral equation (3.13), which can be integrated with help of Monte Carlo methods. Although the Green's function $G(\mathbf{R}', \mathbf{R}, t)$ is not known, it can be approximated for small values of the argument t , and then equation (3.13) can be solved step by step

$$f(\mathbf{R}, t + \Delta t) = \int G(\mathbf{R}, \mathbf{R}', \Delta t) f(\mathbf{R}', t) d\mathbf{R}' \quad (3.14)$$

For further convenience let us split the Hamiltonian into three operators

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3, \quad (3.15)$$

where

$$\begin{aligned} \hat{H}_1 &= -D\Delta, \\ \hat{H}_2 &= D((\vec{\nabla}\vec{F}) + \vec{F}\vec{\nabla}), \\ \hat{H}_3 &= E_L(\mathbf{R}) - E \end{aligned} \quad (3.16)$$

and let us introduce the corresponding Green's functions

$$G_i(\mathbf{R}, \mathbf{R}', t) = \langle \mathbf{R} | e^{-\hat{H}_i t} | \mathbf{R}' \rangle, \quad i = 1, 2, 3 \quad (3.17)$$

The exponential operator can be approximated as (the error comes from the non-commutativity of the \hat{H}_i 's, $i = 1, 2, 3$)

$$e^{-\hat{H}t} = e^{-\hat{H}_1 t} e^{-\hat{H}_2 t} e^{-\hat{H}_3 t} + O(t^2) \quad (3.18)$$

This formula, rewritten in coordinate representation, gives approximation for the Green's function

$$G(\mathbf{R}, \mathbf{R}', t) = \int \int G_1(\mathbf{R}, \mathbf{R}_1, t) G_2(\mathbf{R}_1, \mathbf{R}_2, t) G_3(\mathbf{R}_2, \mathbf{R}', t) d\mathbf{R}_1 d\mathbf{R}_2$$

To obtain the three Green's functions one must solve the differential equations

$$\left\{ \begin{array}{l} -\frac{\partial}{\partial t} G(\mathbf{R}, \mathbf{R}', t) = H_i G(\mathbf{R}, \mathbf{R}', t), \quad i = 1, 2, 3 \\ G(\mathbf{R}, \mathbf{R}', 0) = \delta(\mathbf{R} - \mathbf{R}') \end{array} \right. \quad (3.19)$$

The equation for the kinetic term has the form

$$-\frac{\partial G_1(\mathbf{R}, \mathbf{R}', t)}{\partial t} = -D \Delta G_1(\mathbf{R}, \mathbf{R}', t) \quad (3.20)$$

This is the diffusion equation with diffusion constant $D = \hbar^2/2m$ and its solution is a Gaussian

$$G_1(\mathbf{R}, \mathbf{R}', t) = (4\pi Dt)^{3N/2} \exp\left(-\frac{(\mathbf{R} - \mathbf{R}')^2}{4Dt}\right) \quad (3.21)$$

The equation for the drift force term is

$$-\frac{\partial G_2(\mathbf{R}, \mathbf{R}', t)}{\partial t} = -D \vec{\nabla}(\vec{F} G_2(\mathbf{R}, \mathbf{R}', t)) \quad (3.22)$$

and its solution is

$$G_2(\mathbf{R}, \mathbf{R}', t) = \delta(\mathbf{R} - \mathbf{R}(t)), \quad (3.23)$$

here $\mathbf{R}(t)$ is the solution of the classical equation of motion

$$\begin{cases} \frac{d\mathbf{R}(t)}{dt} = DF(\mathbf{R}(t)), \\ \mathbf{R}(0) = \mathbf{R}' \end{cases} \quad (3.24)$$

The last equation from (3.19) has trivial solution, which describes the *rate term*

$$G_3(\mathbf{R}, \mathbf{R}', t) = \exp((E - E_L(\mathbf{R}))t) \delta(\mathbf{R} - \mathbf{R}') \quad (3.25)$$

3.1.4 DMC algorithm

If the wavefunction of the system $f(\mathbf{R}, t)$ is real and positive, as it happens in case of ground state of a bose system, it can be treated as population density distribution¹

$$f(\mathbf{R}, t) = \sum_{i=1}^{N_W} C \delta(\mathbf{R} - \mathbf{R}_i(t)), \quad (3.26)$$

here C is a positive constant, $\mathbf{R}_i(t)$ are coordinates of a population element (so called *walker*) in $3N$ -dimensional configuration space, $f(\mathbf{R}, t) d\mathbf{R}$ gives the probability to find a walker at time t in vicinity $d\mathbf{R}$ of point \mathbf{R} .

Let us now interpret the action of the each of the three terms of the Hamiltonian (3.15) on the population distribution or, being the same, the action of the corresponding Green's functions (3.21, 3.23, 3.25). In terms of Markov Chains the Green's function is the $G(\mathbf{R}, \mathbf{R}', t)$ is the transition matrix which determines the evolution of the distribution (see eq.(3.14)).

The first term means *diffusion* of each of the walkers in configuration space

¹The formula (3.26) should be understood in the statistical sense, the average of any value A over the l.h.s. and r.h.s distributions are equal to each other in the limit when size of the population N_W tends to infinity $\int A(\mathbf{R}) f(\mathbf{R}, t) d\mathbf{R} = \lim_{N_W \rightarrow \infty} \int A(\mathbf{R}) \sum_{i=1}^{N_W} C \delta(\mathbf{R} - \mathbf{R}_i(t)) d\mathbf{R}$

$$\mathbf{R}^{(1)}(t + \Delta t) = \mathbf{R}(t) + \chi, \quad (3.27)$$

here χ is a random value from a gaussian distribution $\exp(-\chi^2/(4D\Delta t))$.

The second term describes the action of the drift force, which guides the walkers to places in the configuration space, where the trial wavefunction is maximal. This is the way how importance sampling acts in this algorithm.

$$\mathbf{R}^{(2)}(t + \Delta t) = \mathbf{R}(t) + \Delta t DF(\mathbf{R}) \quad (3.28)$$

The corresponding Green's functions of these two steps (3.21 - 3.23) are normalized to one $\int G(\mathbf{x}, \mathbf{x}', t) d\mathbf{x} = 1$. The normalization of wavefunction f is then conserved meaning that the number of walkers remains constant.

The third term is the *branching term*

$$f^{(3)}(\mathbf{R}, t + \Delta t) = \exp(-(E_L(\mathbf{R}) - E)\Delta t) f(\mathbf{R}, t) \quad (3.29)$$

Here the corresponding Green's function (3.25) is no longer normalized and, when the quantity in the exponent is negative (i.e. large values of local energy), then the density of population decreases and vice-versa.

3.1.5 Parallel DMC algorithm

The simulation of a homogeneous infinite system is done by repeating periodically in space the "simulation box" with side L . Such a substitution leads to correlation in space for distances $r > L/2$. It means that the one-body density matrix, the

pair distribution functions, can be calculated only for $r < L/2$. In some cases it is important to have information about the large-scale properties of the system. For example this happens in the region close to the phase transition, where the correlation length is large. In our case we need to find the asymptotic value of the one-body density matrix and as a result it is necessary to use large L . The problem is that doubling the number of particles N at a constant density $n = N/L^3$ enlarges the size of the box only $\sqrt[3]{2} = 1.26$ times, while the time of the calculation scales quadratically. This makes the calculation heavy and one of the possible way out consists in using the parallel computations.

The Diffusion Monte Carlo algorithm can be parallelized in a natural way. In the algorithm the wavefunction f is treated as the density of the probability distribution of walkers (see (3.26)). The walkers explore the coordinate space moving according to (3.27, 3.28), and then some of the walkers are removed or added during the branching process (3.29). The key point is that the walkers move absolutely independently, and consequently can be evaluated on different processors independently.

Here is the list of corrections to the serial calculation:

1. walkers move in space according to (3.27, 3.28), done in parallel
2. the local energy of each walker is calculated, done in parallel
3. other quantities different from energy are calculated (if necessary), done in parallel
4. averages over all walkers are calculated, the regeneration coefficient (3.29) is calculated for each walker and walkers are redistributed among the processors to keep the load constant

The explained above algorithm of numerical simulations produces very high productivity, because all heavy calculations are done in the parallel regime and only

few, like the the balance load, are done in the non-parallel way. Although one also should consider the loss of time due to communication and data transfer between the processes, but amount of this time is negligible in comparison to the length of the calculation.

This parallel algorithm is called *distributed-system method*, another way to build the program is described by the *replicated-system method*[23], which has 5% higher performance.

Monte Carlo methods are very robust to numerical errors and this makes their usage very advantageous. For example, the MC run on a cluster of computers can survive even if one of the processes is switched off during the computation. This will lead only to a decrease in statistics at this step and different loading distribution at the next one. Many other methods, like the direct solution of the differential equation, will break down in a case of such an event.

3.2 Homogeneous Bose Gas

In this section we apply the DMC algorithm to the study of a homogeneous Bose gas modeled by hard spheres.

3.2.1 Trial Wavefunction

The trial wavefunction ψ_T should be chosen as close to the true wave function ψ of the system as possible. If we were able to approximate the system wavefunction with satisfying accuracy, then the sampling over the corresponding distribution (for example with the help of Metropolis algorithm) would give us all properties of the system. However, the problem is that very often it is impossible to find the wavefunction of the system using analytical methods. Here enters the Diffusion Monte Carlo method, which compensates our lack of knowledge and corrects the trial wavefunction provid-

ed that the projection of the trial wavefunction on the true system wavefunction of the system differs from zero.

As the use of the trial wavefunction lies at the heart of the method, it has to be expressed in a way that is fast to calculate or it has to be tabulated.

The common way to construct many-body wavefunctions is to use the Jastrow function consisting of the product of an uncorrelated state and a correlation factor, which is a product of two-body wavefunctions.

$$\psi_T = \prod_i \phi(\vec{r}_i) \prod_{i < j} g(\vec{r}_i, \vec{r}_j) \quad (3.30)$$

The one-body term describes the effect of an external field and is absent in the case of a homogeneous system. For a homogeneous system the trial wavefunction can be written in general as

$$\psi_T(r_1, \dots, r_N) = \prod_{\substack{i=1 \\ j=1}}^N g(|\vec{r}_i - \vec{r}_j|) \quad (3.31)$$

Since we are mainly interested to dilute system a possible way to obtain the pair function $g(r)$ is through the solution of the two-body Schrödinger equation.

$$\left(-\frac{\hbar^2}{2\mu} \Delta + V(\vec{r}) \right) g = \mathcal{E}g, \quad (3.32)$$

here $\mu = m_1 m_2 / (m_1 + m_2) = 2m$ is the reduced mass and r is the interparticle distance. Let's search for the $l = 0$ solution in spherical coordinates

$$-\frac{\hbar^2}{2\mu} \left(g'' + \frac{2}{r} g' \right) + V(r)g = \mathcal{E}g \quad (3.33)$$

The particles are modeled by hard spheres of diameter a and the interaction potential is

$$V(\mathbf{r}) = \begin{cases} +\infty, & |r| \leq a \\ 0, & |r| > a \end{cases} \quad (3.34)$$

The dimensionless Schrödinger equation is obtained by expressing all distances in units of a and energy in units of $\hbar^2/(2ma^2)$

$$\begin{cases} g(x) = 0, & |x| \leq 1 \\ g'' + \frac{2}{x}g' - 2Eg = 0, & |x| > 1 \end{cases} \quad (3.35)$$

So, it is necessary to solve the differential equation

$$\begin{cases} g'' + \frac{2}{x}g' - 2Eg = 0 \\ g(1) = 0 \end{cases} \quad (3.36)$$

The solution of equation (3.36) is $g(x) = A \sin \left(\sqrt{2E}(x-1) \right) / x$, where A is an arbitrary constant.

In dilute systems for small interparticle distance r the correlation factor is well approximated by the function $g(r)$, i.e. by the wavefunction of a pair of particles in vacuum. At large distances the pair wavefunction should be constant, which corresponds to uncorrelated particles.

Taking these facts into account let us introduce the trial function in the following way [24]

$$g(x) = \begin{cases} \frac{A}{x} \sin(\sqrt{2E}(x-1)), & |x| \leq R \\ 1 - B \exp\left(-\frac{x}{\alpha}\right), & |x| > R \end{cases} \quad (3.37)$$

This function has to be smooth at the matching point R , i.e.

1) the $f(x)$ must be continuous

$$\frac{A}{R} \sin(\sqrt{2E}(R-1)) = 1 - B \exp\left(-\frac{R}{\alpha}\right) \quad (3.38)$$

2) its derivative $f'(x)$ must be continuous

$$-\frac{A}{R^2} \sin(\sqrt{E}(R-1)) + \frac{A\sqrt{2E}}{R} \cos(\sqrt{2E}(R-1)) = \frac{B}{\alpha} \exp\left(-\frac{R}{\alpha}\right) \quad (3.39)$$

3) the local energy $E_L(x) = \psi_T^{-1} \hat{H} \psi_T$ must be continuous

$$2E = \frac{\left(\frac{1}{\alpha^2} - \frac{2}{R\alpha}\right) B \exp\left(-\frac{R}{\alpha}\right)}{1 - B \exp\left(-\frac{R}{\alpha}\right)} \quad (3.40)$$

The solution of this system is

$$\begin{cases} A = \frac{R}{\sin(u(1-1/R))} \frac{\xi^2 - 2\xi}{\xi^2 - 2\xi + u^2}, \\ B = \frac{u^2 \exp(\xi)}{\xi^2 - 2\xi + u^2}, \end{cases} \quad (3.41)$$

where we used the notation $u = \sqrt{2E}R$ and $\xi = R/\alpha$. The value of ξ is obtained from the equation

$$1 - \frac{1}{R} = \frac{1}{u} \operatorname{atan} \frac{u(\xi - 2)}{u^2 + \xi - 2} \quad (3.42)$$

There are three conditions for the determination of five unknown parameters, consequently two parameters are left free. The usual way to define them is minimize the variational energy in Variational Monte Carlo which yields an optimized trial wavefunction.

3.2.2 Comparison between VMC and DMC methods

The Jastrow trial-wavefunction obtained in the previous section gives a very good approximation for the ground state wavefunction of dilute Bose gases. One can appreciate this by comparing the VMC and DMC energies (Fig. 3.1). On this plot the relative error $\Delta E/E$ of the energy estimate is presented as a function of the density. The coincidence of DMC and VMC results is very good in the density region $n < 10^{-4}$ and remains quite good for higher densities.

The energy obtained in VMC is always larger than the ground state energy (see Fig. 3.1). In other words, variational simulations always give an *upper bound* to the ground state energy.

$$E^{VMC} \geq E \quad (3.43)$$

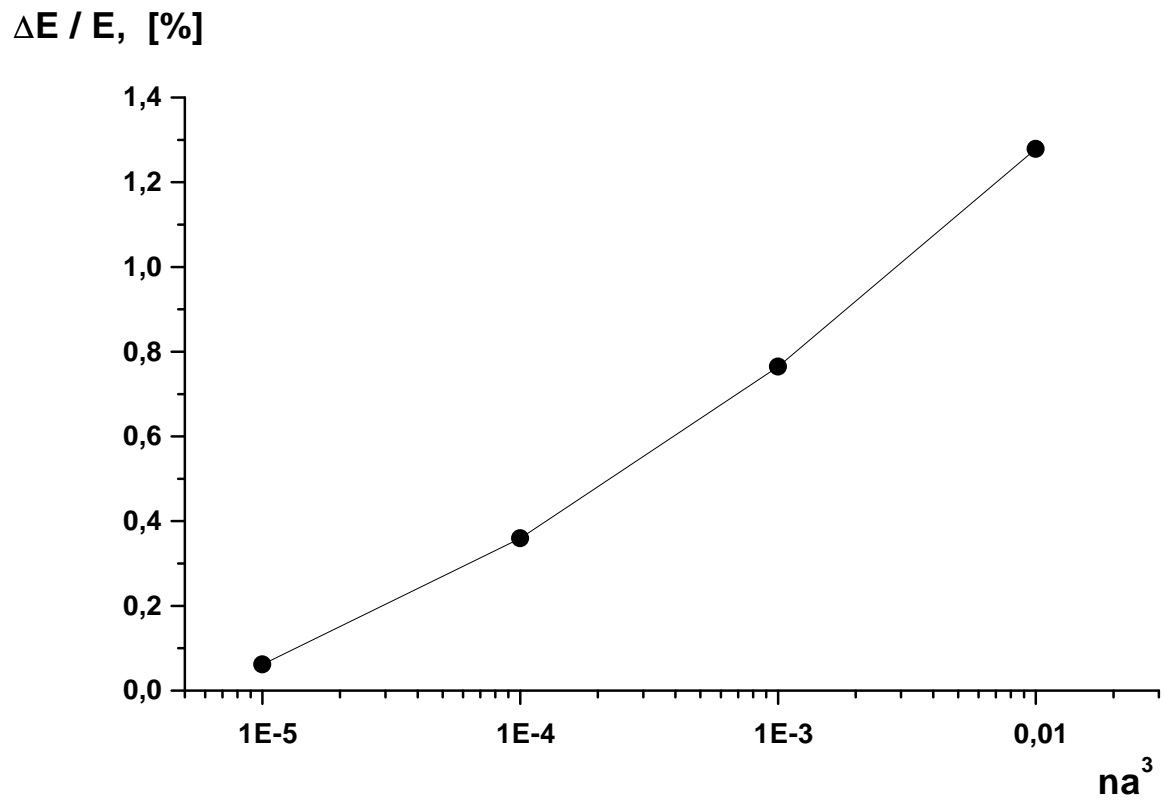


Figure 3.1: Energy comparison between VMC and DMC calculations $\Delta E = E^{VMC} - E^{DMC}$ at different densities na^3

3.3 Outputs of the calculation

The advantage of Diffusion Monte Carlo with respect to usual Variational Monte Carlo methods is that it provides the possibility to calculate pure estimators, which have no bias due to the choice of the trial wave function. This is true for such important quantities as the energy, radial distribution function and superfluid density. For other quantities such as the one body density matrix the DMC method provides mixed estimator which, used in correction with outputs of VMC calculations, allows one to reduce the bias of the trial wavefunction.

3.3.1 Energy

The energy is a direct output of the DMC algorithm. In fact, the population of walkers is stable only if the energy shift E is equal to the value of ground state energy.

The ground state energy can be expressed as an integral ratio

$$E_0 = \frac{\int \psi_T(\mathbf{R}) \hat{H} \phi_0(\mathbf{R}) d\mathbf{R}}{\int \psi_T(\mathbf{R}) \phi_0(\mathbf{R}) d\mathbf{R}}, \quad (3.44)$$

where $\phi_0(\mathbf{R})$ is the ground state eigenfunction of the Hamiltonian $\hat{H} \phi_0(\mathbf{R}) = E_0 \phi_0(\mathbf{R})$.

By multiplying and dividing the integrand in the numerator by $\psi_T(\mathbf{R})$, the formula (3.44) can be rewritten as

$$E_0 = \frac{\int \psi_T^{-1}(\mathbf{R}) \hat{H} \psi_T(\mathbf{R}) \psi_T(\mathbf{R}) \phi_0(\mathbf{R}) d\mathbf{R}}{\int \psi_T(\mathbf{R}) \phi_0(\mathbf{R}) d\mathbf{R}} \quad (3.45)$$

The average of the Hamiltonian over the trial wavefunction is the local energy (see definition (3.10)). Since in the large time limit the distribution function f is proportional to the product of the trial and the ground-state wavefunctions (see eq.

(3.5))

$$\lim_{t \rightarrow \infty} f(\mathbf{R}, t) = c_0 \psi_T(\mathbf{R}) \phi_0(\mathbf{R}, t) \quad (3.46)$$

The calculation of the mean local energy of the walkers provides the value of the ground state energy¹

$$E_0 = \frac{\int E_L(\mathbf{R}) f(\mathbf{R}) d\mathbf{R}}{\int f(\mathbf{R}) d\mathbf{R}} = \frac{1}{N_W} \sum_{i=1}^{N_W} E_L(\mathbf{R}_i) \quad (3.47)$$

3.3.2 Superfluid density

The normal and superfluid fractions of a liquid can be obtained by measuring the momenta of inertia of a rotating bucket. Consider a liquid which is inserted between two cylindrical walls of radii R and $R + d$. If $d \ll R$ then the system can be described as moving between two planes. Let us denote by E_v the ground state energy of the system in equilibrium with the walls which move with velocity v and E_0 the ground state energy of the system at rest. The difference between the energies E_v and E_0 is due to the superfluid component, which remains immobile in contrast to the normal component which is carried along by the moving walls. Thus, the superfluid fraction ρ_s/ρ can be defined as

$$\frac{Nm v^2}{2} \frac{\rho_s}{\rho} = E_v - E_0 \quad (3.48)$$

¹In real DMC simulations the upper limit of the integrals is truncated by $L/2$. The “tail” energy, which is small and is typically much less than 1% of the total energy can be approximated by the formula $E_{tail} = n \int_{L/2}^{\infty} E_L(r) 4\pi r^2 dr$. The idea is that at large distances, where the integral is evaluated, one can safely assume uniform distribution of particles.

Let us introduce the wave-functions f_0 and f_v related to the wave-functions of the system in the reference frames at rest and in motion.

$$f_0(\mathbf{R}, t) = \psi_T(\mathbf{R})\phi_0(\mathbf{R}, t), \quad (3.49)$$

$$f_v(\mathbf{R}, t) = \psi_T(\mathbf{R})\phi_v(\mathbf{R}, t) \quad (3.50)$$

These wavefunctions satisfy the Schrödinger equation with the following Hamiltonians

$$\hat{H}_0 = \frac{1}{2m} \sum_i (-i\hbar \nabla_i)^2 + V(\mathbf{R}) \quad (3.51)$$

for the reference frame at rest and

$$\hat{H}_v = \frac{1}{2m} \sum_i (-i\hbar \nabla_i - m\vec{v})^2 + V(\mathbf{R}) \quad (3.52)$$

for the reference frame at moving with velocity v .

In the reference frame at rest one has

$$-\frac{\partial}{\partial t} f_0(\mathbf{R}, t) = -\frac{\hbar^2}{2m} \sum_{i=1}^N \left[\Delta_i f_0(\mathbf{R}, t) - \nabla_i \left(\vec{F} f_0(\mathbf{R}, t) \right) \right] + (E_L(\mathbf{R}) - E_0) f_0(\mathbf{R}, t) \quad (3.53)$$

The Schrödinger equation in the moving frame is instead

$$\begin{aligned}
-\frac{\partial}{\partial t}f_v(\mathbf{R},t) = & -\frac{\hbar^2}{2m}\sum_{i=1}^N\left[\Delta_i f_v(\mathbf{R},t) - \nabla_i(\vec{F}f_v(\mathbf{R},t))\right] + (E_L(\mathbf{R}) - E_v)f_v(\mathbf{R},t) + \\
& + \frac{Nm v^2}{2}f_v(\mathbf{R},t) + \sum_{i=1}^N i\hbar \vec{v} \nabla_i f_v(\mathbf{R},t) - \frac{i\hbar}{2}\vec{v}\vec{F}f_v(\mathbf{R},t)
\end{aligned} \tag{3.54}$$

Looking at (3.53) and (3.54) it is easy to write the Bloch equations for the Green's functions in the rest frame $G_0(\mathbf{R}, \mathbf{R}', t)$ and in the moving frame $G_v(\mathbf{R}, \mathbf{R}', t)$

$$-\frac{\partial}{\partial t}G_0(\mathbf{R}, \mathbf{R}', t) = \left(-\frac{\hbar^2}{2m}\sum_{i=1}^N\left[\Delta_i - (\nabla_i \vec{F}) - \vec{F} \nabla_i\right] + E_L(\mathbf{R}) - E_0 \right) G_0(\mathbf{R}, \mathbf{R}', t) \tag{3.55}$$

and

$$\begin{aligned}
-\frac{\partial}{\partial t}G_v(\mathbf{R}, \mathbf{R}', t) = & \left(-\frac{\hbar^2}{2m}\sum_{i=1}^N\left[\Delta_i - (\nabla_i \vec{F}) - \vec{F} \nabla_i\right] + E_L(\mathbf{R}) - E_0 + \frac{Nm v^2}{2} \right) G_v(\mathbf{R}, \mathbf{R}', t) + \\
& + \left(\sum_{i=1}^N i\hbar \vec{v} \nabla_i - \frac{i\hbar}{2}\vec{v}\vec{F} \right) G_v(\mathbf{R}, \mathbf{R}', t)
\end{aligned} \tag{3.56}$$

In general the wavefunction $\psi(\mathbf{R}, t)$ of the system satisfies the Schrödinger equation (3.2) and its evolution in time is described by

$$\psi(\mathbf{R}, t) = e^{-(\hat{H}-E)t}\psi(\mathbf{R}, 0) \tag{3.57}$$

The wavefunctions f evolves in time as

$$f(\mathbf{R}, t) = e^{-At}f(\mathbf{R}, 0) \tag{3.58}$$

so, substitution of (3.49) or (3.50) into (3.58) gives

$$\psi_T(\mathbf{R})\psi(\mathbf{R}, t) = e^{-At}\psi_T(\mathbf{R})\psi(\mathbf{R}, 0) \quad (3.59)$$

Combining together (3.57) and (3.59) one has

$$e^{-At} = \psi_T(\mathbf{R})e^{-(\hat{H}-E)t}\psi_T^{-1}(\mathbf{R}) = B e^{-(\hat{H}-E)t} B^{-1}, \quad (3.60)$$

where the operator B is defined as $B|\psi\rangle = \sum_{\mathbf{R}} \psi(\mathbf{R}) \langle \mathbf{R}|\psi\rangle |\mathbf{R}\rangle$.

Let us calculate the trace of the Green's function. From (3.60) it follows that the trace T of the Green's function is equal to

$$T = \int G_0(\mathbf{R}, \mathbf{R}, t) d\mathbf{R} = \int \langle \mathbf{R}|e^{-tA}|\mathbf{R}\rangle d\mathbf{R} = \int \langle \mathbf{R}|B e^{-t(\hat{H}-E)B^{-1}}|\mathbf{R}\rangle d\mathbf{R} \quad (3.61)$$

Here it is possible to use the permutation property of the trace $\text{tr}(AB) = \text{tr}(BA)$

$$T = \int \langle \mathbf{R}|e^{-t(\hat{H}-E)}|\mathbf{R}\rangle d\mathbf{R} \quad (3.62)$$

This formula means that the trace of the Green's function is unaffected by the presence of the trial wavefunction ψ_T .

$$T = \sum_{k,l} \int \langle \mathbf{R}|\phi_k\rangle \langle \phi_k|e^{-t(\hat{H}-E)}|\phi_l\rangle \langle \phi_l|\mathbf{R}\rangle d\mathbf{R} = \sum_k e^{-(E_k-E)t} \quad (3.63)$$

After long enough time of evolution the traces of the Green's function G_0 is fixed by the ground state energy

$$\int G_0(\mathbf{R}, \mathbf{R}, t) d\mathbf{R} \rightarrow e^{-E_0 t}, \quad t \rightarrow \infty, \quad (3.64)$$

Approximation (3.64) is valid for times t such that

$$t \gg 1/E_0 \quad (3.65)$$

Analogously, the trace of $G_v(\mathbf{R}, \mathbf{R}, t)$ is fixed by the ground state energy E_v in the moving frame

$$\int G_v(\mathbf{R}, \mathbf{R}, t) d\mathbf{R} \rightarrow e^{-tE_v} \quad t \rightarrow \infty, \quad (3.66)$$

The Green's function has to comply with periodic boundary conditions, i.e. it must remain the same if one of the arguments is shifted by the period \vec{L}

$$G_0(\vec{r}_1, \dots, \vec{r}_i + \vec{L}, \dots, \vec{r}_N, \mathbf{R}', t) = G_0(\vec{r}_1, \dots, \vec{r}_i, \dots, \vec{r}_N, \mathbf{R}', t), \quad (3.67)$$

$$G_v(\vec{r}_1, \dots, \vec{r}_i + \vec{L}, \dots, \vec{r}_N, \mathbf{R}', t) = G_v(\vec{r}_1, \dots, \vec{r}_i, \dots, \vec{r}_N, \mathbf{R}', t) \quad (3.68)$$

Let us define a new Green's function $\tilde{G}(\mathbf{R}, \mathbf{R}', t)$ in such a way that

$$G_v(\mathbf{R}, \mathbf{R}', t) = \exp\left(i \frac{m}{\hbar} \vec{v} \sum_i (\vec{r}_i - \vec{r}_i')\right) \tilde{G}(\mathbf{R}, \mathbf{R}', t) \quad (3.69)$$

The Green's function $\tilde{G}(\mathbf{R}, \mathbf{R}', t)$ satisfies the same Bloch equation (3.55) as $G_0(\mathbf{R}, \mathbf{R}', t)$, but the boundary conditions differ from (3.67, 3.68) by the presence of a phase factor

$$\tilde{G}(\vec{r}_1, \dots, \vec{r}_i + \vec{L}, \dots, \vec{r}_N, \mathbf{R}', t) = \exp\left(-i \frac{m}{\hbar} \vec{v} \vec{L}\right) \tilde{G}(\vec{r}_1, \dots, \vec{r}_i, \dots, \vec{r}_N, \mathbf{R}', t), \quad (3.70)$$

Results (3.64) and (3.66) give the following relation

$$\frac{\int \tilde{G}(\mathbf{R}, \mathbf{R}, t) d\mathbf{R}}{\int G_0(\mathbf{R}, \mathbf{R}, t) d\mathbf{R}} = \frac{\int G_v(\mathbf{R}, \mathbf{R}, t) d\mathbf{R}}{\int G_0(\mathbf{R}, \mathbf{R}, t) d\mathbf{R}} \approx \frac{e^{-tE_v}}{e^{-tE_0}} \quad (3.71)$$

By assuming that $t(E_v - E_0) \ll 1$ one gets

$$\frac{e^{-tE_v}}{e^{-tE_0}} \approx 1 - t(E_v - E_0) \quad (3.72)$$

The ratio of the traces is related to the energy difference

$$\frac{\int \tilde{G}(\mathbf{R}, \mathbf{R}, t) d\mathbf{R}}{\int G_0(\mathbf{R}, \mathbf{R}, t) d\mathbf{R}} = 1 - t(E_v - E_0) \quad (3.73)$$

The Green's function \tilde{G} coincides with G_0 apart when the boundary conditions are invoked. Let us introduce the *winding number* W [25], which counts how many times the boundary conditions were used during the time evaluation

$$1 - t(E_v - E_0) = \frac{\int |f(\mathbf{R}, t)|^2 e^{-i \frac{m}{\hbar} \vec{v} W \vec{L}} d\mathbf{R}}{\int |f(\mathbf{R}, t)|^2 d\mathbf{R}} \quad (3.74)$$

In the case of slowly moving walls, i.e. when $\vec{v} \frac{m}{\hbar} W \vec{L} \ll 1$, the exponential can be expanded in a Taylor series

$$e^{-i\frac{m}{\hbar}\vec{v}W\vec{L}} \approx 1 - i\frac{m}{\hbar}\vec{v}W\vec{L} - \frac{m^2}{\hbar^2}(\vec{v}W\vec{L})^2 \quad (3.75)$$

Let us define W through the distance the particles have gone during the time t

$$W\vec{L} = \sum_{i=1}^N (\vec{r}_i(t) - \vec{r}_i(0)) \quad (3.76)$$

The average value of the linear term is equal to zero and the final result is

$$\frac{\rho_s}{\rho} = \frac{2m}{\hbar^2} \frac{1}{6N} \lim_{t \rightarrow \infty} \frac{1}{t} \frac{\int |f(\mathbf{R}, t)|^2 (WL)^2 d\mathbf{R}}{\int |f(\mathbf{R}, t)|^2 d\mathbf{R}} \quad (3.77)$$

An interpretation of this result is that the superfluid fraction is equal to the ratio between the diffusion constant D_v of the center of the mass of the system and the free diffusion constant D_0 ¹

$$\frac{\rho_s}{\rho} = \frac{D_v}{D_0}, \quad (3.78)$$

where the diffusion constants are defined as

$$D_0 = \frac{\hbar^2}{2m}, \quad (3.79)$$

$$D_v = \lim_{t \rightarrow \infty} \frac{N}{6t} \frac{\int f(\mathbf{R}, t) \left(\vec{R}_{CM}(t) - \vec{R}_{CM}(0) \right)^2 d\mathbf{R}}{\int f(\mathbf{R}, t) d\mathbf{R}}, \quad (3.80)$$

¹It is necessary to note that here the “diffusion” occurs in imaginary time and it has nothing to do with diffusion in real space.

where the center of the mass of the system is

$$\vec{R}_{CM}(t) = \frac{1}{N} \sum_{i=1}^N \vec{r}_i(t) \quad (3.81)$$

By calculating the ratio D_v/D_0 as a function of time one finds that this ratio starts from 1 at small time step, decreases and finally reaches a constant plateau, In practice the best way of finding the asymptotic value is to fit the ration D_v/D_0 with the function $C_0 + C_1(1 - \exp(-C_2 t))/t$, where C_0 , C_1 , C_2 are fitting parameters [26].

It is worth to remind that the calculation of ρ_s/ρ is independent of the choice of the trial wave-function and similarly to the calculation of energy the superfluid fraction is a pure estimator.

3.3.3 One body density matrix and condensate fraction

The one body density matrix (OBDM) of a homogeneous system described by the many body wavefunction $\psi(r_1, \dots, r_N)$ is defined as follows

$$\rho(|\vec{r}' - \vec{r}''|) = N \frac{\int \dots \int \phi_0^*(\vec{r}', \vec{r}_2, \dots, \vec{r}_N) \phi_0(\vec{r}'', \vec{r}_2, \dots, \vec{r}_N) d\vec{r}_2 \dots d\vec{r}_N}{\int \dots \int |\phi_0(\vec{r}_1, \dots, \vec{r}_N)|^2 d\vec{r}_1 \dots d\vec{r}_N}. \quad (3.82)$$

Since in DMC calculation one can not sample the ground-state probability distribution ϕ_0^2 , instead one samples the mixed probability $\psi_T \phi_0$ and one can calculate the mixed one-body density matrix

$$\rho_{mixed}(r) = N \frac{\int \dots \int \psi_T^*(\vec{r}'' + \vec{r}, \vec{r}_2, \dots, \vec{r}_N) \phi_0(\vec{r}'', \vec{r}_2, \dots, \vec{r}_N) d\vec{r}_2 \dots d\vec{r}_N}{\int \dots \int \psi_T^*(\vec{r}_1, \dots, \vec{r}_N) \phi_0(\vec{r}_1, \dots, \vec{r}_N) d\vec{r}_1 \dots d\vec{r}_N}, \quad (3.83)$$

This formula can be further developed

$$\begin{aligned}
\rho_{mixed}(r) &= N \frac{\int \dots \int \psi_T^*(\vec{r}_1 + \vec{r}, \vec{r}_2, \dots, \vec{r}_N) \phi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \delta(\vec{r}_1 - \vec{r}'') d\vec{r}_1 \dots d\vec{r}_N}{\int \dots \int \psi_T^*(\vec{r}_1, \dots, \vec{r}_N) \phi_0(\vec{r}_1, \dots, \vec{r}_N) d\vec{r}_1 \dots d\vec{r}_N} = \\
&= n \frac{\int \dots \int [\psi_T^*(\vec{r}_1 + \vec{r}, \vec{r}_2, \dots, \vec{r}_N) (\psi_T^*(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N))^{-1}] f(\vec{r}_1, \dots, \vec{r}_N) d\vec{r}_1 \dots d\vec{r}_N}{\int \dots \int f(\vec{r}_1, \dots, \vec{r}_N) d\vec{r}_1 \dots d\vec{r}_N}, \quad t \rightarrow \infty
\end{aligned} \tag{3.84}$$

where we have used the asymptotic formula (3.46). If the trial wavefunction is chosen as a product of pair functions (see eq. (3.31) then using the notation $\mu(|\vec{r}_i - \vec{r}_j|) = \ln g(|\vec{r}_i - \vec{r}_j|)$ one has

$$\psi_T(\vec{r}_1, \dots, \vec{r}_N) = \prod_{i < j} e^{\mu(|\vec{r}_i - \vec{r}_j|)} \tag{3.85}$$

Then, the ratio of trial wavefunction appearing in (3.84) becomes

$$\begin{aligned}
\frac{\psi_T(\vec{r}_1 + \vec{r}, \dots, \vec{r}_N)}{\psi_T(\vec{r}_1, \dots, \vec{r}_N)} &= \prod_{j>1} \exp(\mu(|\vec{r}_1 + \vec{r} - \vec{r}_j|) - \mu(|\vec{r}_1 - \vec{r}_j|)) = \\
&= \exp\left(\sum_{j>1} \mu(|\vec{r}_1 + \vec{r} - \vec{r}_j|) - \mu(|\vec{r}_1 - \vec{r}_j|)\right).
\end{aligned} \tag{3.86}$$

In order to gain better statistics one can average over all particles

$$\frac{1}{N} \sum_{i=1}^N \frac{\psi_T(\vec{r}_1, \dots, \vec{r}_i + \vec{r}, \dots, \vec{r}_N)}{\psi_T(\vec{r}_1, \dots, \vec{r}_N)} = \frac{1}{N} \sum_{i=1}^N \exp\left(\sum_{j \neq i}^N \mu(|\vec{r}_i + \vec{r} - \vec{r}_j|) - \mu(|\vec{r}_i - \vec{r}_j|)\right)$$

The asymptotic limit of the OBDM gives the condensate density

$$\lim_{r \rightarrow \infty} \rho(r) = \frac{N_0}{V} \tag{3.87}$$

and the condensate fraction is obtained by the calculating the asymptotic ratio

$$\lim_{r \rightarrow \infty} \frac{\rho(r)}{\rho} = \frac{N_0}{N} \quad (3.88)$$

3.3.4 Extrapolation technique from mixed and variational estimators

The one body density matrix (3.84) corresponds to a mixed estimator, when the averaging of the variable A is done in an asymmetric way $\langle \phi_0 | \hat{A} | \psi_T \rangle$. If the trial wavefunction is close to the true ground-state wavefunction ϕ_0 one can estimate the ground-state average $\langle \phi_0 | \hat{A} | \psi_0 \rangle$ by using the following technique.

Let us denote the difference between the trial wave function and ground-state wave function as $\delta\psi$

$$\phi_0 = \psi_T + \delta\psi \quad (3.89)$$

Then the ground-state average can be written as

$$\langle \phi_0 | \hat{A} | \phi_0 \rangle = \langle \psi_T | \hat{A} | \psi_T \rangle + 2\langle \phi_0 | \hat{A} | \delta\psi \rangle + \langle \delta\psi | \hat{A} | \delta\psi \rangle \quad (3.90)$$

If $\delta\psi$ is small the second order term $\langle \delta\psi | \hat{A} | \delta\psi \rangle$ can be neglected. After substitution $\langle \phi_0 | \hat{A} | \delta\psi \rangle = \langle \psi_T | \hat{A} | \phi_0 \rangle - \langle \psi_T | \hat{A} | \psi_T \rangle$ the extrapolation formula becomes

$$\langle A \rangle = \langle \phi_0 | \hat{A} | \phi_0 \rangle = 2\langle \phi_0 | \hat{A} | \psi_T \rangle - \langle \psi_T | \hat{A} | \psi_T \rangle \quad (3.91)$$

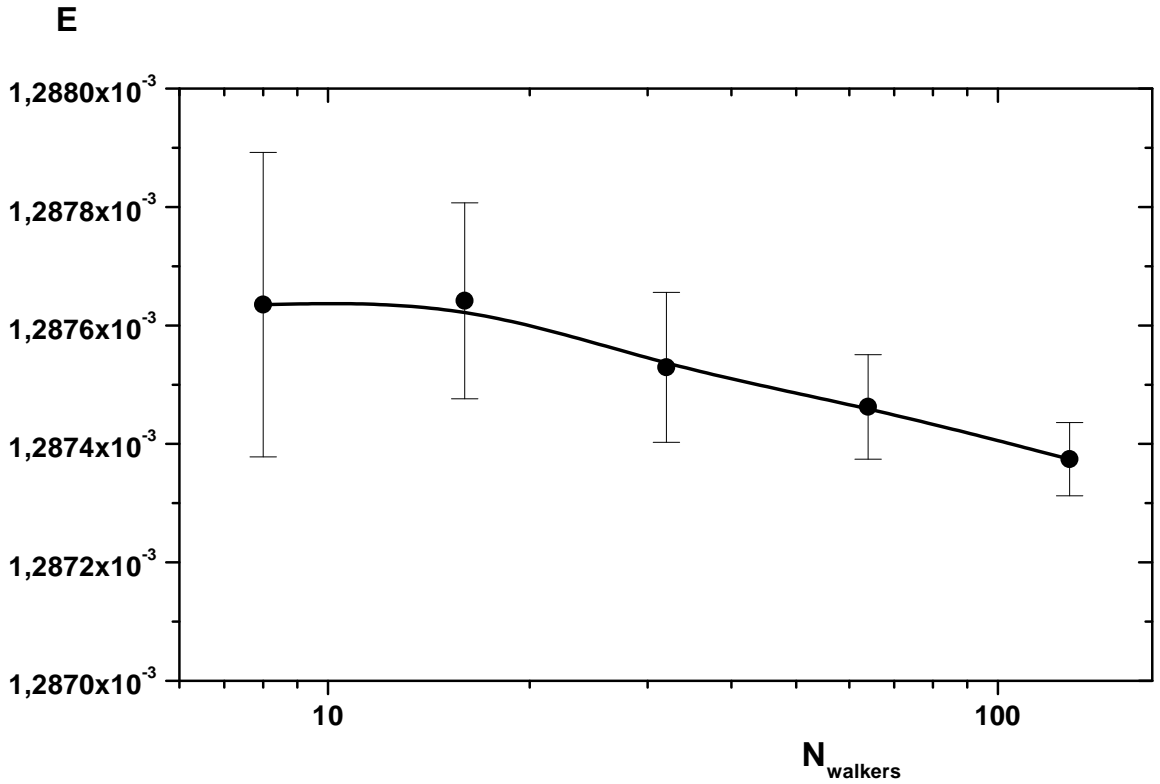


Figure 3.2: Hard-spheres at $na^3 = 10^{-4}$. Dependence of the energy on the size of the population of walkers.

3.4 Systematic errors

3.4.1 Population of walkers

A key ingredient of the DMC algorithm is the branching process (3.29). The algorithm is exact, i.e. gives the exact ground-state energy of the system, in the limit of an infinite population of walkers. However it is necessary to understand how many walkers have to be used in practice to estimate the energy with a given value of accuracy [27].

In Fig. 3.2 we plot the energy for a given value of the density $na^3 = 10^{-4}$ as a function of the mean number of walkers. In all simulations carried out in this work we have used about one hundred walkers.

3.4.2 Time step

The approximation (3.18) of the Green's function has first order accuracy in the timestep. High order approximations can be used. One of the possibilities to gain second order accuracy is to use the formula

$$e^{-\hat{H}t} = e^{-\hat{H}_3 t/2} e^{-\hat{H}_2 t/2} e^{-\hat{H}_1 t} e^{-\hat{H}_2 t/2} e^{-\hat{H}_3 t/2} + O(t^3) \quad (3.92)$$

The result for the energy in the DMC algorithm depends on the value of the timestep used. The exact ground-state energy is obtained by extrapolating the results to the zero timestep. Approximation (3.92) for the evaluation operator leads to a quadratic dependence of the energy on the timestep. The result of such a calculation is presented in Fig. 3.3. In this respect the use of a quadratic algorithm, such as (3.92), is preferable because for small timestep the results are less sensitive to the choice of the timestep and with a judicious choice one does not need to extrapolate.

On one side the timestep has to be small so that the approximation in the Green's function is good, on the other side the larger is the timestep the faster the phase space is explored and less number of iterations are needed for the same statistical accuracy.

3.4.3 Finite size errors

The standard way to simulate infinite systems is to use a finite box with periodic boundary conditions. As a result, if the size of the box is not large enough, one can have large errors due to finite size effects. These effects are very important in the proximity of a phase transition.

In our simulations finite size effects are well under control, as is evident from Fig.3.4, and few tens of particles are enough to properly simulate the system in the thermodynamic limit.

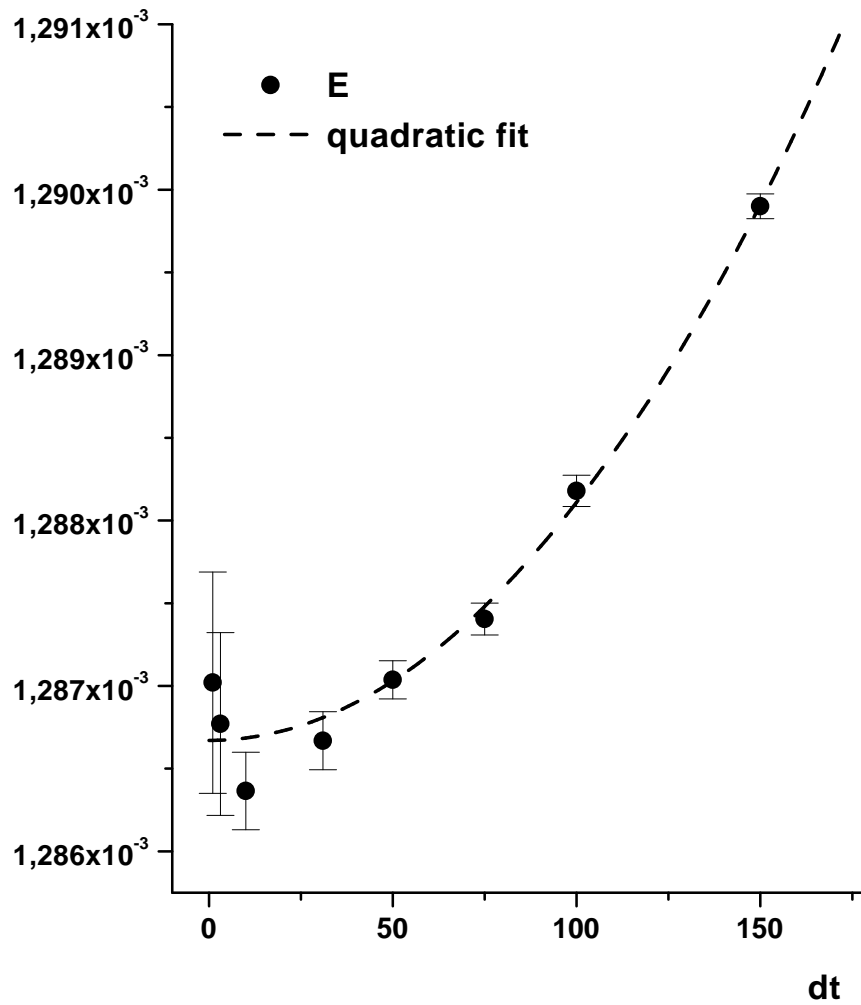


Figure 3.3: Hard spheres at $na^3 = 10^{-4}$. Dependence of the energy on the time step.

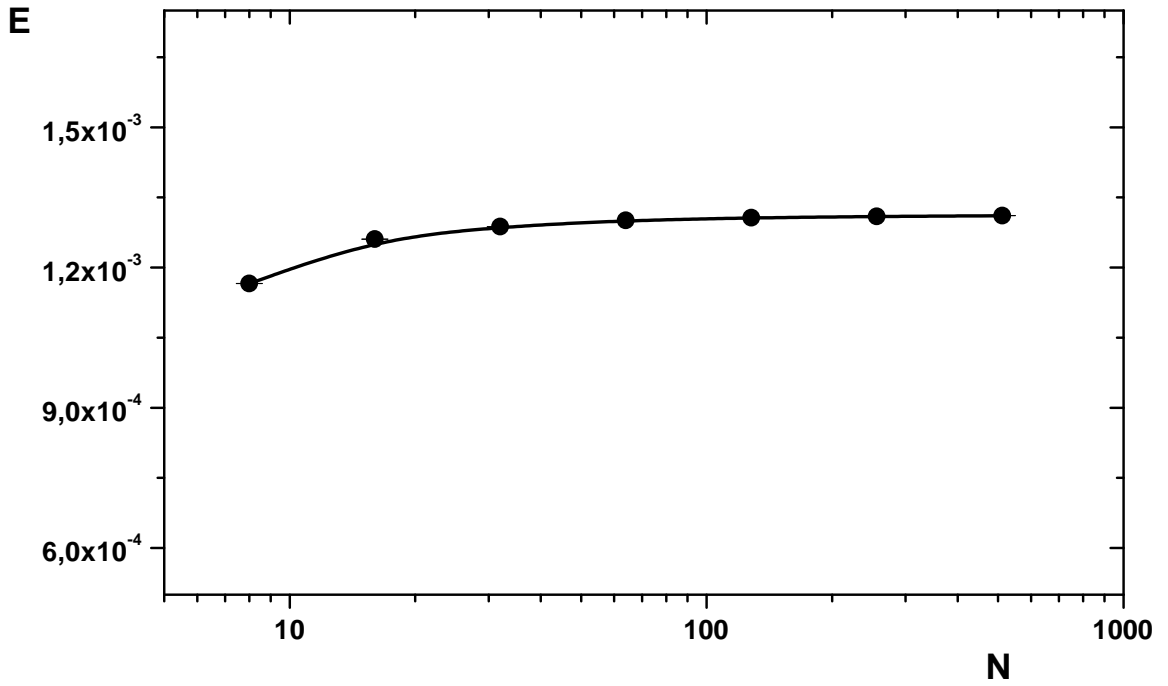


Figure 3.4: Dependence of the energy E measured in DMC simulation on the size of the system N

3.4.4 Other sources of errors

Another type of error comes from the bias due to the trial wave function. For the quantities measured as pure estimators no effect was found. Also in the case of other estimators, such as the OBDM, the use of an optimized trial wavefunction yields reasonably small differences between mixed and variational estimators (less than 10%). In this case we believe that the extrapolated technique of section 3.3.4 gives reliable results.

There is another source of error which arises from the hard-sphere model. In the DMC method the particles propagate according to diffusion (3.27) and drift (3.28) moves. Due to finite timestep it can happen during the simulation that some particle overlap with an impurity or another particle. This walker should not contribute to the calculation of averages because it does not satisfy the boundary conditions of the problem. One possibility is to artificially eliminate the walker or to redo the last

diffusion jump so that it will choose another trajectory. Both of the choices bring in a systematic error. It is hard to investigate the effect of this error because it comes always mixed up with the timestep errors (3.4.2) and it is impossible to separate two effects. It is clear however that the percentage of the restarted or removed walkers must be kept small. For example in our calculations this percentage was always smaller than few percent.

Chapter 4

Dilute Bose gas with disorder: a Diffusion Monte Carlo study

4.1 Introduction

The problem of bosons in the presence of disorder has generated much theoretical and experimental interest.

The superfluid fraction in liquid ^4He has been measured for different types of adsorbing porous media. In vycor, which has small ($\approx 70 \text{ \AA}$) pores and porosity of 30% the superfluid transition is considerably suppressed, but exhibits the same critical exponent as in the bulk [7]. In contrast, in aerogel, which is characterized by larger pores with a broad distribution of sizes and porosity 85 – 99.5%, the superfluid transition is changed by only a few milli-kelvins while the critical exponents are quite different from the bulk [9, 10]. Some experimental studies have also investigated, by measuring the dynamic structure factor, the nature of the elementary excitations in these systems [28] and the role played by the condensate fraction [29].

Theoretical studies of these effects have been proposed, mostly concerning models on a lattice. Many of the theoretical works address the problem of the superfluid-

insulator transition and the critical behavior near the phase transition [30, 8, 31]. The boson localization and the structure of the Bose-glass phase have also been investigated.

Quantum Monte Carlo techniques have been used for numerical simulations of the disordered Bose systems at low temperatures. Most of them concern systems on a lattice using the Bose-Hubbard or equivalent models. These studies have been carried out in 1D [32], 2D [21, 33, 34] and 3D [35, 36] both at zero and finite temperatures. The structure of the phase diagram has been investigated and the properties of the superfluid, Mott insulator and Bose-glass phase have been addressed.

There are very few simulations of disordered boson systems in the continuum. In ref. [37] the effect of impurities on the excitation spectrum in liquid ^4He is investigated using PIMC. The same technique is applied to study the effect of disorder on the superfluid transition in a Bose gas [38].

We apply DMC to study a hard-sphere Bose gas at zero temperature in the presence of hard-sphere quenched impurities. Hard sphere quenched impurities are easy to implement in a numerical simulation and provide a reasonable model for liquid ^4He in the porous media. Another possible physical realization of this model is given by trapped gases in the presence of heavy impurities.

The free parameters in our simulations are:

- the density of the particles na^3 , where a is the diameter of the hard-sphere particle scattering length,
- the concentration of impurities $\chi = N^{imp}/N$ fixed by the ratio of the number of impurities to the number of particles used in the simulation,
- the ratio b/a , where $b = R^{imp} + a/2$ with R^{imp} radius of the hard-sphere impurity.

The same parameters (2.9) were used in the perturbative analysis discussed previously (see section 2.2.1).

The goals of our study are:

- recover the “weak” disorder regime where the results of perturbation theory apply,
- verify the scaling behavior of the effects due to disorder in terms of the single parameter $R = \chi (b/a)^2$ as predicted from the Bogoliubov model
- understand if one can realize situations where the superfluid density is smaller than the condensate fraction
- investigate if within our model there exists a quantum phase transition for strong disorder

4.2 Trial wavefunction

The trial wavefunction for the pure system was constructed in chapter 3.2.1. In this section the same approach will be extended to systems in the presence of quenched impurities.

The wave function of the system is chosen as the product of one-body and two-body wavefunctions.

$$\psi_T(\vec{r}_1, \dots, \vec{r}_N) = \prod_{\substack{i=1, N \\ j=1, N}} f_{PP}(|\vec{r}_i - \vec{r}_j|) \prod_{\substack{i=1, N \\ j=1, N_{imp}}} f_{PI}(|\vec{r}_i - \vec{r}_j^{imp}|), \quad (4.1)$$

where f_{PP} stands for the particle-particle wavefunction, which has already been obtained in section 3.2.1 and is defined by (3.37), (3.41) and (3.42). In eq. (4.1) f_{PI} describes the effect of the impurities on each particle.

To construct f_{PI} we use a similar procedure as for f_{PP} , i.e. we solve the particle-impurity Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\Delta + V_{PI}(\vec{r})\right) f = \mathcal{E}f, \quad (4.2)$$

where the reduced particle-impurity mass is equal to the mass of a particle, because the quenched impurity is infinitely massive. Let us look for the symmetric solution in spherical coordinates

$$-\frac{\hbar^2}{2m}\left(f'' + \frac{2}{r}f'\right) + V_{PI}(r)f = \mathcal{E}f \quad (4.3)$$

The particle is modeled by a hard sphere of diameter a and the impurity by a hard sphere of diameter $2b - a$. The particle-impurity interaction potential is

$$V_{PI}(r) = \begin{cases} +\infty, & |r| \leq b \\ 0, & |r| > b \end{cases} \quad (4.4)$$

where b is the particle-particle s -wave scattering length

The dimensionless Schrödinger equation has form (lengths in units of a and energies in units of $\hbar^2/(2ma^2)$)

$$\begin{cases} f(x) = 0, & |x| \leq b/a \\ f'' + \frac{2}{x}f' - Ef = 0, & |x| > b/a \end{cases} \quad (4.5)$$

and the differential equation which has to be solved is

$$\begin{cases} f'' + \frac{2}{x}f' - Ef = 0 \\ f\left(\frac{b}{a}\right) = 0 \end{cases} \quad (4.6)$$

The solution is $f(x) = A \sin(\sqrt{E}(x - b/a)) / x$, with A being an arbitrary constant.

Let us construct the particle-impurity wave function f_{PI} in the same way as it was done for the particle-particle wavefunction. We introduce a matching point R_{PI} and choose

$$f_{PI}(x) = \begin{cases} \frac{A}{x} \sin\left(\sqrt{E}\left(x - \frac{b}{a}\right)\right), & |x| \leq R_{PI} \\ 1 - B \exp\left(-\frac{x}{\alpha}\right), & |x| > R_{PI} \end{cases} \quad (4.7)$$

The function f_{PI} must be smooth at the matching point. The request of continuity for f_{PI} , its derivative f'_{PI} and the local energy $E_L(R) = -(f''_{PI}(R) - 2f'_{PI}(R)/R) / f_{PI}(R)$ is fulfilled

$$\begin{cases} A &= \frac{R_{PI}}{\sin(u(1 - a/bR))} \frac{\xi^2 - 2\xi}{\xi^2 - 2\xi + u^2}, \\ B &= \frac{u^2 \exp(\xi)}{\xi^2 - 2\xi + u^2}, \\ u &= \sqrt{E} R_{PI}, \\ \xi &= R_{PI}/\alpha, \\ 1 - \frac{a}{bR} &= \frac{1}{u} \operatorname{atan} \frac{u(\xi - 2)}{u^2 + \xi - 2} \end{cases} \quad (4.8)$$

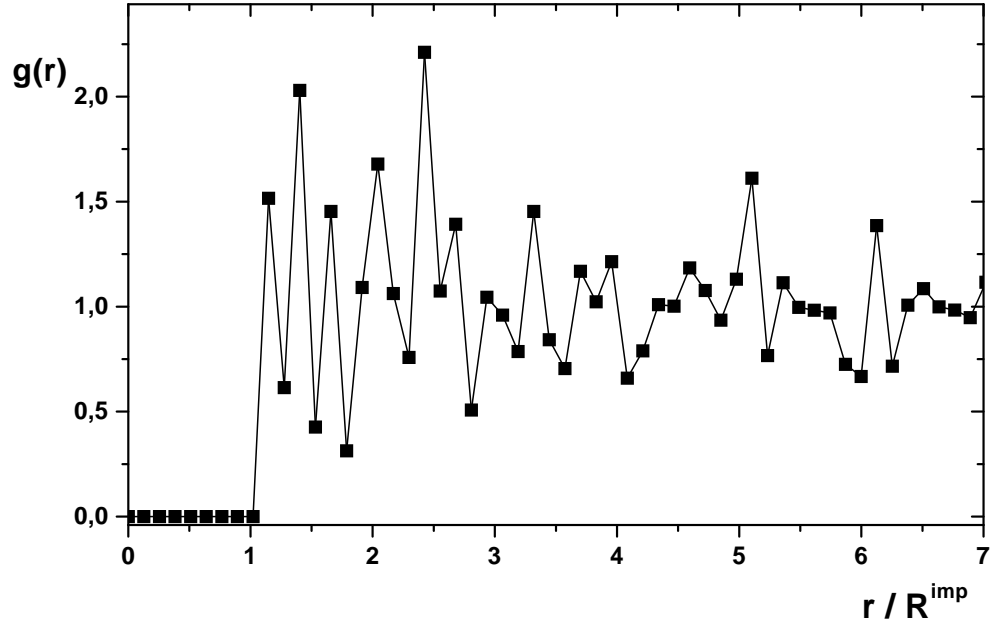


Figure 4.1: Radial distribution function of the impurities for a given one configuration of disorder

4.3 Average over disorder

4.3.1 Distribution of impurities

The positions of the quenched impurities in the simulation box are fixed at the beginning of the simulation run following a uniform random distribution. We also require that the impurities do not overlap. To achieve this we throw the impurities at random within the simulation box and then rethrow all overlapping impurities until the required configuration is obtained. In Fig. 4.1 we show the radial distribution function of a typical configuration of impurities.

$$(E_1 + \dots + E_N) / N$$

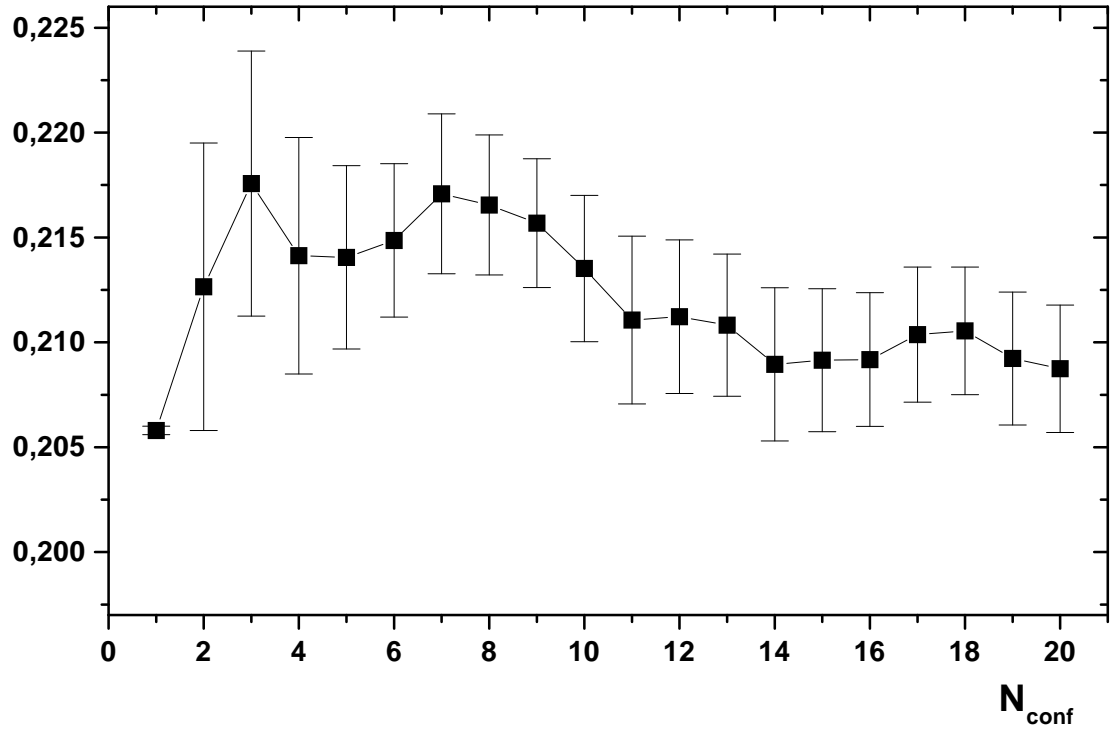


Figure 4.2: The average of the energy over disorder as a function of the number of different disorder realizations. The error bars show the variance of the averaging.

4.3.2 Dependence on the number of disorder realizations

Once the relevant physical quantities (energy, superfluid and condensate fraction) have been calculated for a given configuration of disorder, the simulation is repeated for different configurations and finally the average over disorder configurations is taken.

As the computation for a given disorder configuration is heavy and it takes a lot of time to complete the runs with different configurations, it is very important to understand the behavior of the statistical error due to the average over realizations. The results for the energy are shown in Fig. 4.2.

Fortunately, energy and the other quantities converge very rapidly to the mean value. Due to the self-averaging 5 or 6 disorder configurations are enough for most of

the cases.

4.4 Results

4.4.1 Ground-state energy

The energy of a dilute Bose gas in the presence of impurities is given by result (2.18). It is derived under the assumptions that the gas parameter is small $na^3 \ll 1$ and the external field is weak.

Using the DMC algorithm we investigate the dependence of the ground-state energy both on the density na^3 and on the strength of the disorder $R = \chi(b/a)^2$. The main contribution to the energy comes from the mean-field term (see result (1.14) obtained from the Gross-Pitaevskii equation). In order to better understand the results for the energy it is useful to subtract the mean-field term E_{MN} from the total energy E .

Let us first consider the energy dependence on R . For weak disorder ($R = 2$) the predictions well agree with the results of DMC simulations. By increasing R while keeping na^3 fixed one sees deviation from analytical prediction.

The Bogoliubov model is valid if the gas parameter na^3 is small. Fig. 4.3 shows that the values of the gas parameter where the theoretical prediction holds depends on the strength of disorder. For weak disorder ($R = 2$) agreement is found up to very high densities $na^3 \approx 10^{-2}$. By increasing the amount of disorder deviations appear for smaller values of na^3 . For $R = 12.5$ numerical and analytical results coincide up to $na^3 \approx 5 \cdot 10^{-4}$ and for very strong disorder $R = 100$ no agreement is found at densities $na^3 > 10^{-5}$.

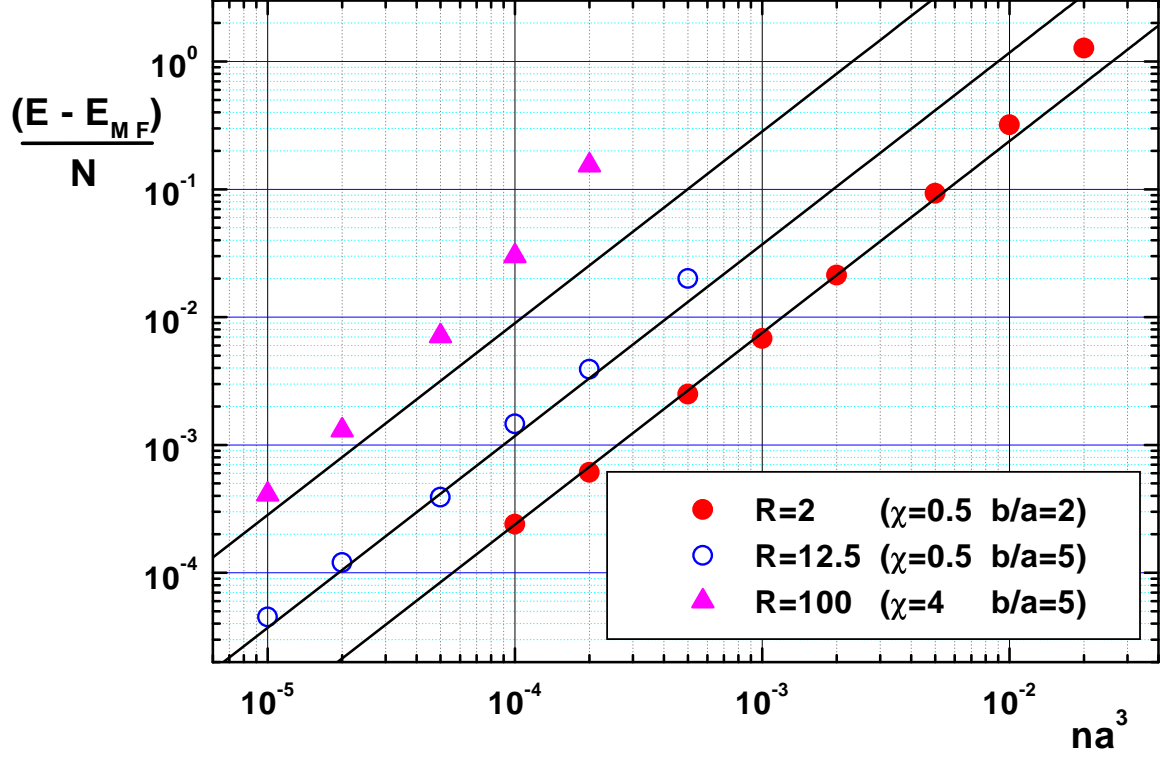


Figure 4.3: Beyond mean-field energy per particle $E - E_{MF}$ as a function of density na^3 for different strengths of disorder R . The solid lines correspond to the analytical prediction (2.18)

4.4.2 Superfluid density and condensate fraction

The predictions of Bogoliubov theory for the condensate and superfluid fraction are given by (2.23) and (2.68). As already mentioned in section 2.3.3 a very interesting consequence of these results is that for any value of na^3 and $R > 5.1$ the superfluid fraction ρ_s/ρ is less than the condensate fraction N_0/N .

We have investigated the dependence of the superfluid and condensate fraction on the density na^3 and the strength of disorder R . The results of the DMC simulations are presented in Fig. 4.4. At low density the DMC results always confirm the predictions of Bogoliubov model, but the region of validity of the model depends on the strength of disorder. If disorder is weak ($R = 2$) the superfluid fraction is described correctly up to density $na^3 \approx 5 \cdot 10^{-3}$ while the condensate fraction starts to deviate much earlier. By increasing disorder we find agreement over a smaller range in density. For $R = 12.5$ the superfluid fraction agrees with the Bogoliubov prediction only up to $na^3 \approx 5 \cdot 10^{-4}$ and the condensate fraction only up to $na^3 \approx 2 \cdot 10^{-4}$. The strength of disorder is here larger than the critical value $R_c = 5.1$ and Bogoliubov model predicts $\rho_s/\rho < N_0/N$. Our results show that the condensate fraction decreases faster than predicted and we do not see this phenomenon. In the presence of very strong disorder $R = 100$ we find no quantitative agreement for $na^3 > 10^{-5}$, at large densities, however, we find $\rho_s/\rho < N_0/N$.

Let us now fix $na^3 = 10^{-4}$ and study the dependence of ρ_s/ρ and N_0/N on the strength of disorder. From Fig. 4.5 one sees that for very weak disorder (i.e. small R) Bogoliubov results are valid. For larger disorder we find deviations. Bogoliubov model predicts a linear dependence on R , with a different slope for ρ_s/ρ and N_0/N . We find instead that the two decrease together up to the strong disorder regime where $\rho_s/\rho < N_0/N$ as in Fig. 4.4.

A different behavior exhibited at the larger density $na^3 = 10^{-2}$ as shown in Fig. 4.6. Even in the pure case ($R = 0$) the condensate fraction does not agree with Bogoliubov

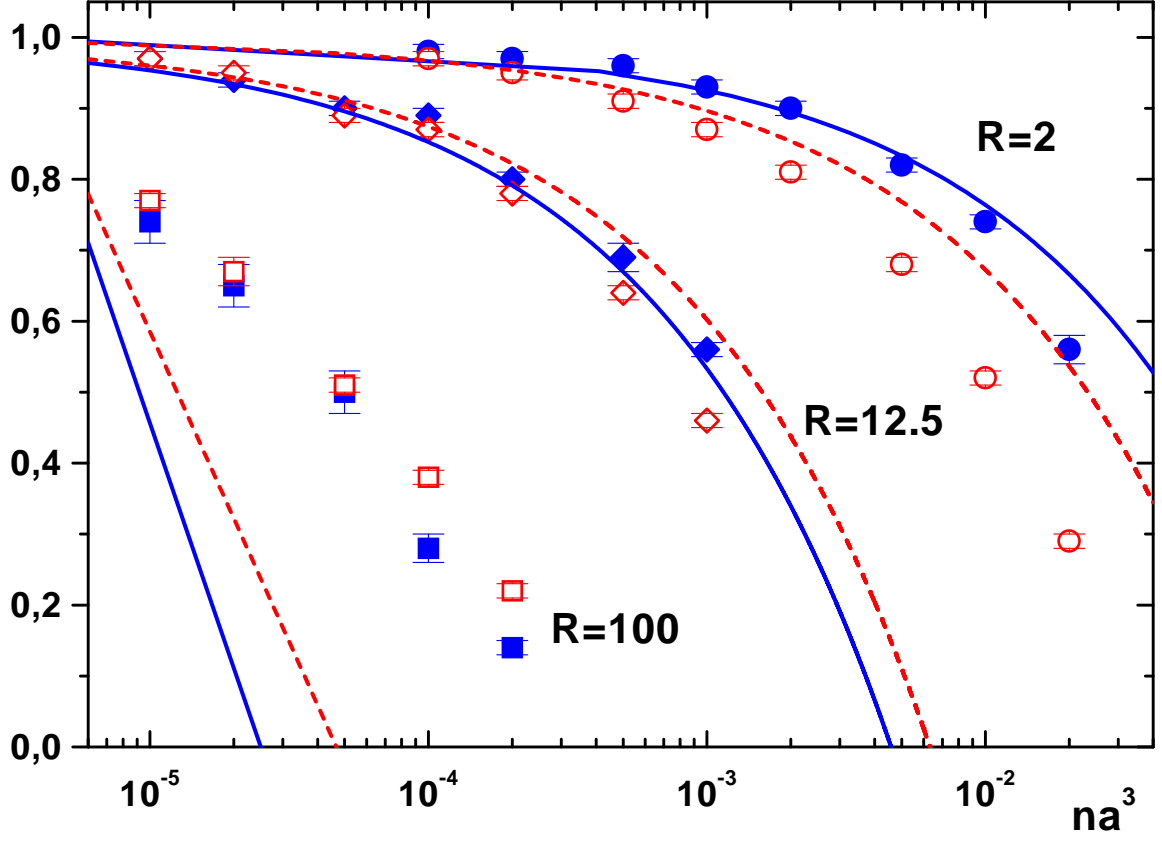


Figure 4.4: Condensate fraction N_0/N (open symbols) and superfluid fraction ρ_s/ρ (solid symbols) as a functions of density na^3 , for $R = 2$, $R = 12.5$, $R = 100$. The solid curve is the Bogoliubov prediction for the superfluid fraction [Eq.(2.68)], the dashed curve for the condensate fraction [Eq.(2.23)].

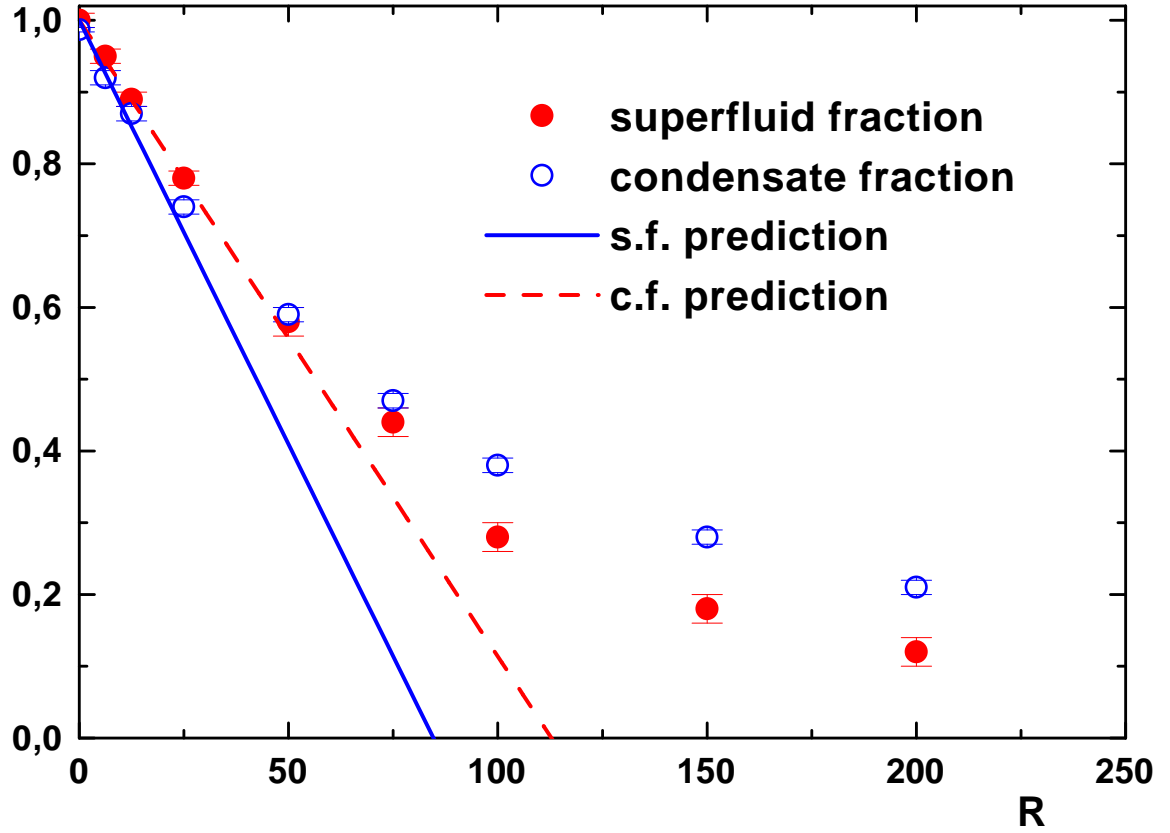


Figure 4.5: Condensate fraction N_0/N and superfluid fraction ρ_s/ρ as a function of $R = \chi(b/a)^2$. Here $na^3 = 10^{-4}$ and $b/a = 5$. The dashed and solid lines show Bogoliubov predictions for N_0/N and ρ_s/ρ respectively.

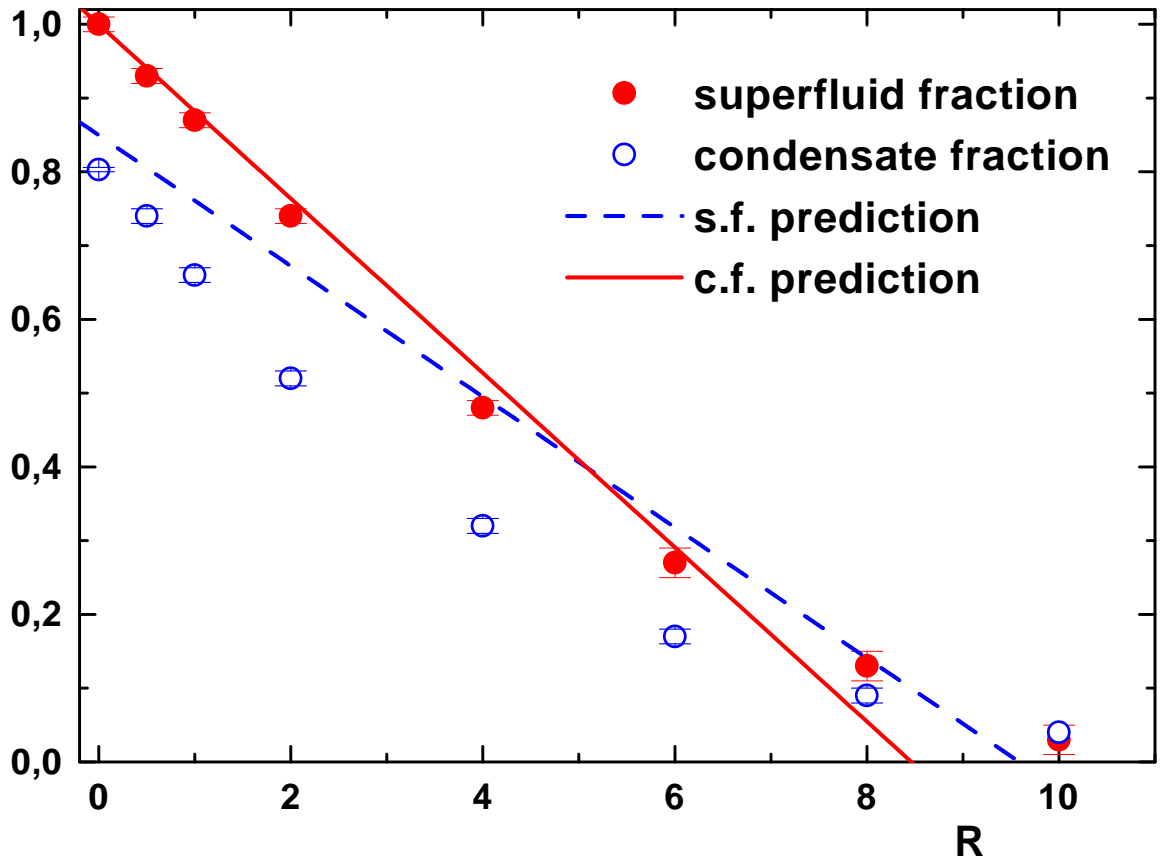


Figure 4.6: Condensate fraction N_0/N and superfluid fraction ρ_s/ρ as a function of $R = \chi(b/a)^2$. Here $na^3 = 10^{-2}$ and $b/a = 2$. The dashed and solid lines show Bogoliubov predictions for N_0/N and ρ_s/ρ respectively.

prediction and by increasing disorder deviations are more evident. On the contrary, the superfluid density well agrees with Bogoliubov prediction.

For small values of R , analogously to the case $na^3 = 10^{-4}$, ρ_s/ρ and N_0/N decrease linearly with a similar slope.

Let us comment on the result $\rho_s/\rho < N_0/N$ which we find for large values of R (see Fig. 4.4 and 4.5). This result is highly unusual since in general¹ $\rho_s/\rho < N_0/N$. For example, in liquid ^4He at low temperatures only 10% of the particles are in the condensate, although the system is entirely superfluid. An extreme example is

¹The only exception[11] known to us takes place in the vicinity of the λ -transition in liquid ^4He , where $N_0 \propto (T_\lambda - T)^{2\beta}$ while $\rho_s \propto (T_\lambda - T)^{(2-\alpha)/3}$, and $2\beta = (2-\alpha)(1-\zeta)/3$ with ζ positive. Still, for ^4He both indices α and ζ are very small, so with very good accuracy $\rho_s \sim N_0 \sim (T_\lambda - T)^{2/3}$ and the difference is so small that there is no hope to measure it experimentally.

provided by two-dimensional Bose systems at $T \neq 0$ which do not exhibit Bose-Einstein condensation (Hohenberg theorem), but do exhibit superfluidity below the Kosterlitz-Thoules transition temperature.

It is interesting to understand how it is possible to realize a system with $\rho_s/\rho < N_0/N$, or even to realize a normal system (i.e. $\rho_s = 0$) with nonzero condensate. A possible answer is by realizing an adsorbing medium with isolated cavities of typical size larger than the healing length. The gas gets trapped in the cavities and a condensate can still exist in each of the cavities, while the overall conductivity is absent. Let us estimate what is the critical value for the excluded volume at which the gas the critical parameters when the fluid can not flow from one side of the box to another (i.e. the percolation threshold). The relative excluded volume for the impurities can be estimated as

$$p = \frac{V^{excl}}{V} = \frac{\frac{4}{3}\pi b^3 N_{imp}}{V} = \frac{4\pi}{3} \chi \left(\frac{b}{a}\right)^3 na^3 \quad (4.9)$$

The percolation threshold is given by $p_c = 0.70$ [39]. In the case of the results of Fig. 4.5 (i.e. $na^3 = 10^{-4}$ and $b/a = 5$) the percolation threshold corresponds to $R_c = 350$. This means that the system is approaching the percolation limit and we can expect that $\rho_s/\rho < N_0/N$.

4.4.3 Scaling behaviour

The strength of disorder is described by two independent parameters: the particle-impurity scattering length b and the concentration $\chi = N^{imp}/N$. One of the important results of the Bogoliubov model is that a single parameter $R = \chi(b/a)^2$ is sufficient to describe the effect of disorder (see eqs. (2.18), (2.23), (2.68)).

We have calculated the condensate and superfluid fraction by changing both b and χ while keeping $R = \chi(b/a)^2$ constant. The results are shown in Fig. 4.7 for

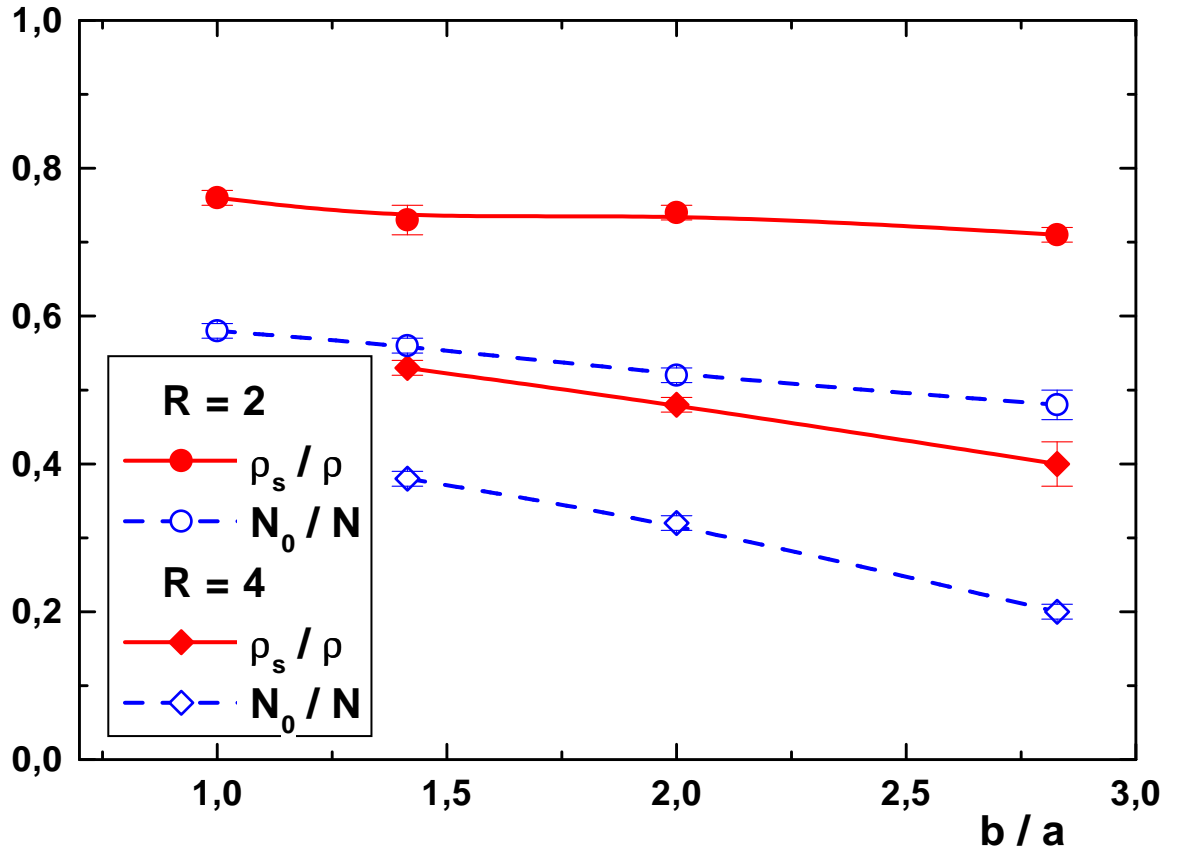


Figure 4.7: Condensate fraction N_0/N and superfluid fraction ρ_0/ρ as functions of impurity size b for two values of the scaling parameter $R = 2$ and $R = 4$, and density $na^3 = 10^{-2}$

$na^3 = 10^{-2}$ and $R = 2, 4$ and in Fig. 4.8 for $na^3 = 10^{-4}$ and $R = 25, 100$.

Both at low and high density we see that the scaling behavior for N_0/N and $\rho_s\rho$ is well satisfied for the smallest values of R ($R = 25$ for $na^3 = 10^{-4}$ and $R = 2$ for $na^3 = 10^{-2}$). It is worth noticing that these values of R and na^3 correspond to regime where the results of first order perturbation theory do not apply (see Figs. 4.5, 4.6). This means that the scaling behavior in the parameter R is valid also beyond the region of applicability of the perturbation expansion.

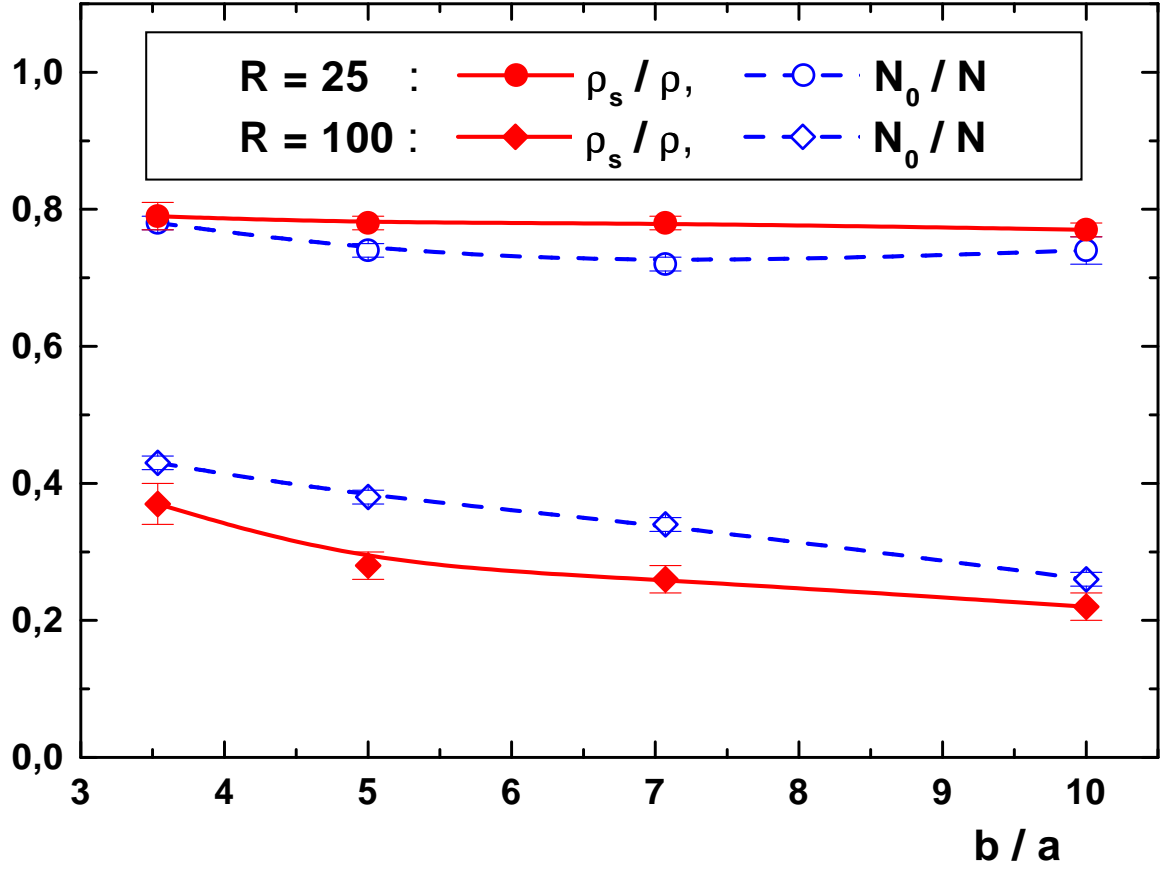


Figure 4.8: Condensate fraction N_0/N and superfluid fraction as functions of impurity size b for fixed value of the scaling parameter $R = 25$ and $R = 100$, and density $na^3 = 10^{-4}$

4.4.4 Shape of the one-body density matrix

The shape of the one-body density matrix (1.45) has been calculated within the Bogoliubov model and is given by (1.47) in the pure system and by (2.25) in the system with disorder. The derivation of these results is valid for dilute systems in the presence of weak disorder, so one expects to find agreement with the DMC results for small values of na^3 and R . Since the Bogoliubov model neglects short-range correlation, we also expect that result (2.25) is valid for large values of r ($r \gg a$, $r \gg b$).

The DMC simulation gives the mixed estimator for the OBDM and the VMC gives the variational estimate. By calculating these results using the extrapolation technique (3.91), we can estimate the pure OBDM.

We have calculated the OBDM at different densities na^3 and for a fixed strength of the disorder $R = 100$. The results are shown in Fig. 4.9. Although the strength of the disorder is large we find good agreement at small densities while by increasing in the density we see significant differences.

4.4.5 Quantum phase transition

By adding disorder to the system the condensate and superfluid density are depleted. One expects that at some critical amount of disorder superfluidity vanishes and the system becomes normal. We want to investigate the quantum phase transition of the hard-sphere gas in the presence of hard-sphere impurities at $T = 0$.

In the vicinity of the phase transition the correlation length becomes large. This means that in the MC simulation one has finite size errors (see 3.4.3) and it is necessary to carry out calculations with systems of different size and finally extrapolate to the thermodynamic limit.

We calculate the superfluid density as a function of the concentration of impurities

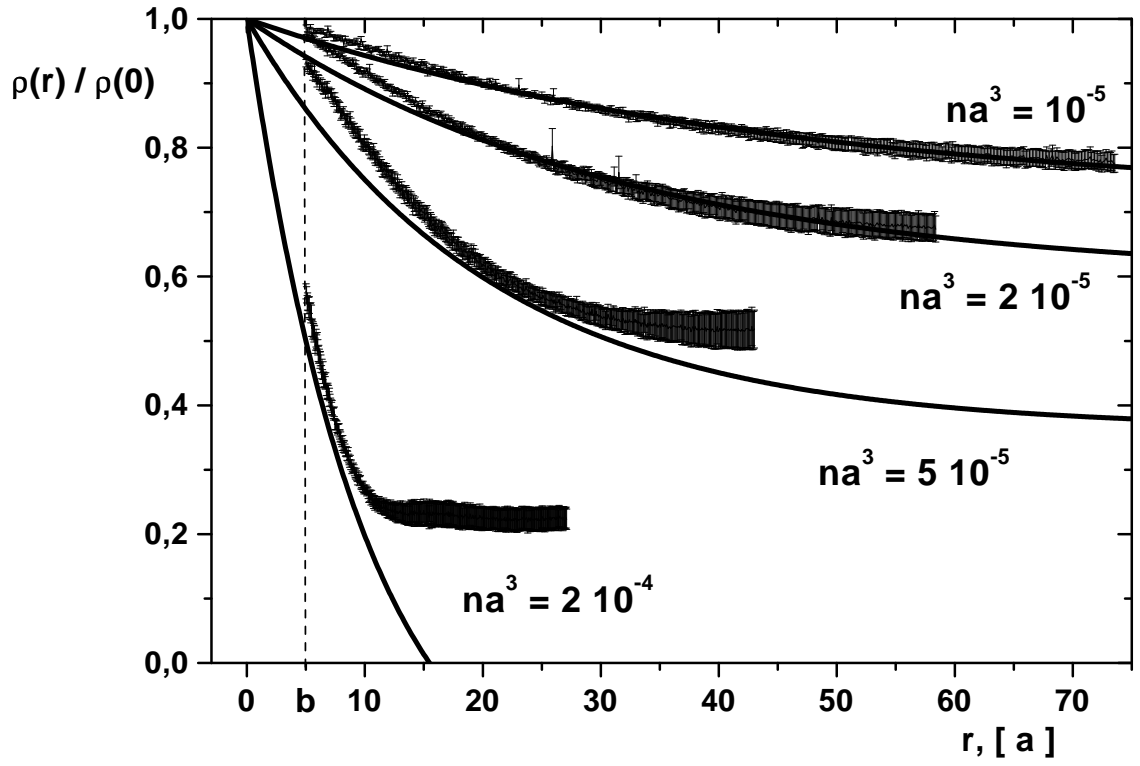


Figure 4.9: One-body density matrix $\rho_s(r)/\rho(0)$ at different densities $na^3 = 10^{-5}, 2 \cdot 10^{-5}, 5 \cdot 10^{-5}, 2 \cdot 10^{-4}$, and $R = \chi(b/a)^2 = 100$ with $b/a = 5$. Solid lines correspond to result (2.25).

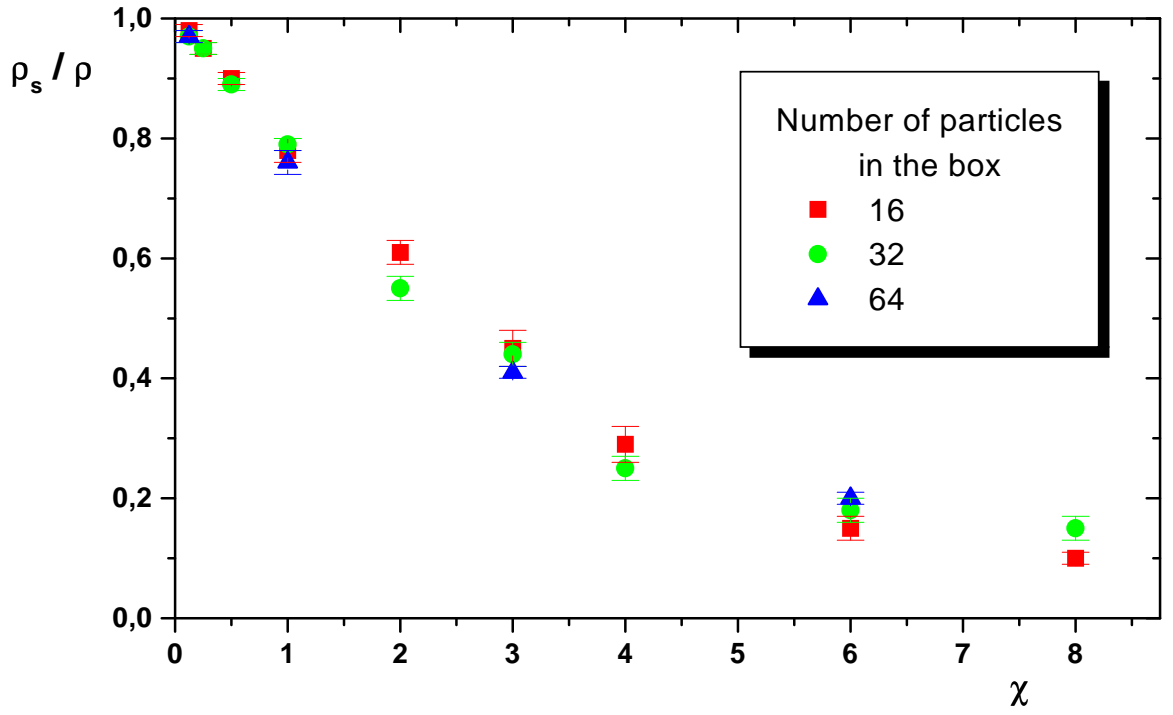


Figure 4.10: Superfluid density measured as a function of χ at density $na^3 = 10^{-4}$ and $b/a = 5$ with 16, 32 and 64 particles in the simulation box

χ while keeping the size of the impurity constant. The simulation is carried out for systems of 16, 32 and 64 particles with periodic boundary conditions. The results for the low density $na^3 = 10^{-4}$ is presented in Fig. 4.10 and for the density $na^3 = 10^{-2}$ in Fig. 4.11.

The figures show that there is no significant finite size effect present which means that we are still far from the critical region.

The further increase of the strength of disorder in Fig. 4.10 and Fig. 4.11 is impossible, because of the constraint of non-overlapping impurities. We conclude that within our model of non-overlapping impurities the superfluid-insulator quantum transition is absent.

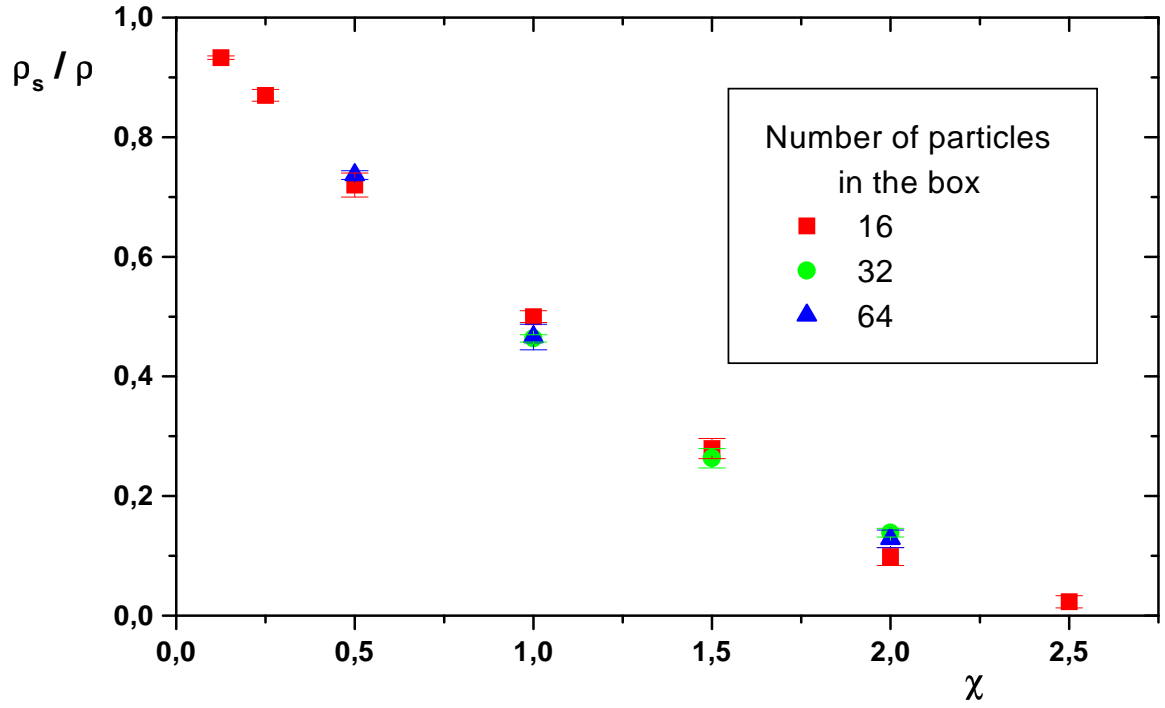


Figure 4.11: Superfluid density measured as a function of χ at density $na^3 = 10^{-2}$ and $b/a = 2$ with 16, 32 and 64 particles in the simulation box

Bibliography

- [1] A. Einstein, Sitzber. Kgl. Preuss. Akad. Wiss. 261 (1924)
- [2] A. Einstein, Sitzber. Kgl. Preuss. Akad. Wiss. 3 (1925)
- [3] F. London, Nature (London) **141**, 632 (1938)
- [4] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor*, Science **269**, 198 (1995)
- [5] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Bose-Einstein condensation in a gas of sodium atoms*, Phys. Rev. Lett. **75**, 3969 (1995)
- [6] F. Dalfovo, S. Giorgini, L. Pitaevskii, S. Stringary, *Theory of Bose-Einstein condensation in trapped gases* Rev.Mod. Phys, **71** 463 (1999)
- [7] John D. Reppy, *Superfluid Helium in Porous Media*, J. Low Temp. Phys, **87** 205 (1992)
- [8] Kanwal G. Singh and Daniel S. Rokhsar, *Disordered bosons: Condensate and excitations*, Phys.Rev.B **49** 9013 (1994)

- [9] G. F. S. Wong, P. A. Crowell, H. A. Cho, and J. D. Reppy, *Superfluid critical behavior in the presence of a dilute correlated impurity*, Phys. Rev. B **48** 3858 (1993)
- [10] I. F. Herbut, *Critical exponents at the superconductor-insulator transition in dirty-boson systems*, Phys.Rev. B, **61**, 14723 (2000)
- [11] E. M. Lifshitz, L. P. Pitaevskii, *Statisticheskaya fizika II*, Moscow, Fiziko-Matematicheskaya Literatura, (in russian) (2000)
E. M. Lifshitz, L. P. Pitaevskii, *Statistical Physics - Part 2*, Pergamon Press, (1980)
- [12] E. P.Gross, Nuovo Cimento **20** 454 (1961)
- [13] E. P.Gross, J. Math. Phys. **4** 195 (1963)
- [14] L. P. Pitaevskii Zh.Eksp.Teor.Fiz. **40** 646 (1961)
Sov.Phys.JETP **13**, 451 (1961)
- [15] N. Bogoliubov, J.Phys. (USSR) **11**, 23 (1947)
- [16] K. Huang, Hsin-Fei Meng *Hard-Sphere Bose Gas in Random External Potentials*, Phys. Rev. Lett. **69** num. 4 p. 644 (1992)
- [17] G. Baym, in *Mathematical Methods in Solid State and Superfluid Theory*, edited by R. C. Clark and G. H. Derrick. Oliver and Boyd, Edinburgh (1969)
- [18] K. Huang, *Bose-Einstein Condensation and Superfluidity*, in *Bose-Einstein Condensation*, edited by A. Griffin, D. W. Snoke, S. Stringari. Cambridge University Press (1995)
- [19] S. Giorgini, L. Pitaevskii, S. Stringari, *Effects of disorder in a dilute Bose gas*, Phys. Rev. B **49** 12938 (1994)

- [20] D. M. Ceperley, *Path integrals in the theory of condensed helium*, Reviews of Modern Physics, **67** 279-355 (1995)
- [21] D. M. Ceperley, E. L. Pollock, *Path-integral simulation of the superfluid transition in two-dimensional ^4He* , Phys.Rev.B **39** 2084 (1989)
- [22] *Path-integral computation of superfluid densities*, E .L. Pollock and D. M. Ceperley Phys.Rev.B **36** 8343 (1987)
- [23] Andrea Bosin, Giuliana Demurtas and Manuela Menchi, *Quantum Monte Carlo simulations on a parallel distributed architecture*, Dipartimento di Scienze Fisiche, University of Cagliari, Italy
- [24] S. Giorgini, J. Boronat, and J. Casulleras, *Ground state of a homogeneous Bose gas: A diffusion Monte Carlo calculation*, Phys. Rev. A **60** 5129 (1999)
- [25] E. L. Pollock and D. M. Ceperley, *Path-integral computation of superfluid densities*, Phys. Rev. B, **36**, 8343 (1987)
- [26] Shiwei Zhang, N.Kawashima, J. Carlson and J. E. Gubernatis, *Quantum Simulations of the Superfluid-Insulator Transition for Two-dimensional, Disordered, Hard-Core-Bosons*, Phys.Rev.Lett **74** 1500 (1995)
- [27] Nicolas Cerf and Oliver C.Martin, *Finite population-size effects in projection Monte Carlo methods*, Phys.Rev.E **51** 3679 (1995)
- [28] O. Plantevin, B. Fak, H. R. Glyde, J. Bossy, J. R. Beamish *Elementary excitations of liquid ^4He in aerogel*, Phys.Rev.B, **57** 10775 (1998)
- [29] H. R. Glyde, O. Plantevin, B. Fak, G. Coddens, P. S. Danielson, and H. Schober, *Dynamics of liquid ^4He in Vycor*, Phys. Rev. Lett. **84** 2646 (2000)

- [30] Matthew P. A. Fisher, Peter B. Weichman, G. Grinstein, and Daniel S. Fisher, *Boson localization and the superfluid-insulator transition*, Phys.Rev.B **40** 546 (1989)
- [31] M. Ma, B. I. Halperin, P. A. Lee, *Strongly disordered superfluids: Quantum fluctuations and critical behavior*, Phys.Rev.B **34** 3136 (1986)
- [32] R. T. Scalettar, G. G. Batrouni, and G. T. Zimanyi, *Localization in Interacting, Disordered, Bose Systems* Phys. Rev. Lett. **66** 3144 (1991)
- [33] S. Zhang and N. Kawashima, *Quantum Simulations of the Superfluid-Insulator Transition for Two-Dimensional, Disordered, Hard-Core Bosons*, Phys. Rev. Lett. **74** 1500 (1995)
- [34] W. Krauth, N. Trivedi, and D. Ceperley *Superfluid-Insulator Transition in Disordered Boson Systems*, Phys. Rev. Lett. **67** 2307 (1991)
- [35] Ying-Hong Li and S. Teitel, *Three-dimensional random XY model: Application to the superfluid transition of ^4He in porous media*, Phys.Rev.B **41** 11388 (1990)
- [36] K. Moon and S. M. Girvin, *Critical Behavior of Superfluid ^4He in Aerogel*, Phys.Rev.Lett. **75** 1328
- [37] M. Boninsegni and H. R. Glyde, *Excitations of liquid ^4He in disorder*, J. Low Temp. Phys. **112** 251 (1998).
- [38] M. C. Gordillo and D. M. Ceperley, *The effect of disorder on the critical temperature of a dilute hard sphere gas*, Phys. Rev. Lett., **85** 4735-4738 (2000);
- [39] R. M. Sok, *Permeation of Small Molecules across a Polymer Membrane: a computer Simulation Study*, University of Groningen

Appendix A

Appendix

A.1 Notation for Fourier transform

$$f(\mathbf{r}) = \int e^{i\mathbf{k}\mathbf{r}} f_k \frac{d\mathbf{k}}{(2\pi)^3} \quad (\text{A.1})$$

$$f_k = \int e^{-i\mathbf{k}\mathbf{r}} f(\mathbf{r}) d\mathbf{r} \quad (\text{A.2})$$

$$\delta\mathbf{k} = \int e^{i\mathbf{k}\mathbf{r}} d\mathbf{r} \quad (\text{A.3})$$

$$\int \delta\mathbf{k} \frac{d\mathbf{k}}{(2\pi)^3} = 1 \quad (\text{A.4})$$

A.2 useful formulae

$$\begin{aligned} E(p) &= \sqrt{\left(\frac{\hbar^2 k^2}{2m} + (mc^2)^2\right)^2 - (mc^2)^2} = \\ &= \sqrt{\left(\frac{p^2}{2m}\right)^2 + (pc)^2} = mc^2 \left(\frac{p}{mc}\right) \sqrt{1 + \frac{1}{4} \left(\frac{p}{mc}\right)^2} \end{aligned} \quad (\text{A.5})$$

$$L_p = \frac{1}{mc^2} \left(E(p) - \frac{p^2}{2m} - mc^2 \right) \quad (\text{A.6})$$

$$\begin{aligned} L_p^2 &= \frac{2E(p)}{(mc^2)^2} \left(E(p) - \frac{p^2}{2m} - mc^2 \right) + 1 = \\ &= \frac{2E(p)}{(mc^2)^2} \left(E(p) - \sqrt{E(p)^2 + (mc^2)^2} \right) + 1 \end{aligned} \quad (\text{A.7})$$

$$\begin{aligned} u_k^2 &= \frac{1}{1 - L_p^2} = \frac{\sqrt{E^2(k) + (mc^2)^2}}{2E(p)} + \frac{1}{2} = \\ &= \frac{p^2/2m + mc^2}{2E(p)} + \frac{1}{2} = \frac{(mc^2)^2}{2E(p) \left(\sqrt{E^2(k) + (mc^2)^2} - E(p) \right)} \end{aligned} \quad (\text{A.8})$$

$$\begin{aligned} v_k^2 &= \frac{L_p^2}{1 - L_p^2} = \frac{\sqrt{E^2(k) + (mc^2)^2}}{2E(p)} - \frac{1}{2} = \\ &= \frac{p^2/2m + mc^2}{2E(p)} - \frac{1}{2} = \frac{(mc^2)^2}{2E(p) \left(\sqrt{E^2(k) + (mc^2)^2} + E(p) \right)} \end{aligned} \quad (\text{A.9})$$

$$u_k v_k = \frac{L_p}{1 - L_p^2} = -\frac{mc^2}{2E(p)} \quad (\text{A.10})$$

$$\frac{1 + L_p}{1 - L_p} = \frac{u_k + v_k}{u_k - v_k} = \frac{\hbar^2 k^2}{2mE(p)} \quad (\text{A.11})$$

Appendix B

Series expansion of the OBDM

The one-body density matrix of the pure system at zero temperature is given by (1.47). One can rewrite this integral as

$$\rho^{(1)}(r) = \frac{na}{\pi r} \int_0^\infty F(\xi) \sin\left(\frac{\xi r}{\sqrt{2}r_0}\right) d\xi \quad (\text{B.1})$$

with the function $F(\xi)$ defined as

$$F(\xi) = 2 \left(1 + \frac{\xi^2}{4}\right)^{1/2} - \left(1 + \frac{\xi^2}{4}\right)^{-1/2} - \xi \quad (\text{B.2})$$

and $r_0 = a/\sqrt{8\pi na^3}$ being the healing length.

Let us integrate (B.1) by parts $2\mathcal{K}$ times. All terms which have the form $\sin(\xi r/\sqrt{2}r_0)F^{(k)}(\xi)\Big|_0^\infty$ disappear, because the sinus function is equal to zero in $\xi = 0$ and $F^{(k)}(\infty) = 0$, terms with cosine contribute $\cos(\xi r/\sqrt{2}r_0)F^{(k)}(\xi)\Big|_0^\infty = -F^{(k)}(0)$. The result of the integration is the following

$$\begin{aligned}\rho^{(1)}(r) = & \frac{na}{\pi r} \sum_{k=0}^{\mathcal{K}} (-1)^k \left(\frac{\sqrt{2}r_0}{r} \right)^{2k+1} F^{(2k)}(0) + \\ & + (-1)^{\mathcal{K}+1} \int_0^{\infty} F^{(2\mathcal{K}+1)}(\xi) \sin \left(\frac{\xi r}{\sqrt{2}r_0} \right) \left(\frac{\sqrt{2}r_0}{r} \right)^{2\mathcal{K}+1} d\xi\end{aligned}\quad (\text{B.3})$$

The k -th derivative of the function F can be calculated from the differentiation of the Taylor expansion of F in zero

$$F^{(2k)}(0) = \frac{1+2k}{1-2k} \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2}-k\right)} \frac{(2k)!}{2^{2k} k!} \quad (\text{B.4})$$

As a result one has a representation of $\rho(r)$ in series of powers of $1/r^2$.

By using the expansion (B.3) one can calculate the leading terms of $\rho^{(1)}(r)$ for $r \rightarrow \infty$

$$\rho^{(1)}(r) = \frac{\sqrt{na}}{2\pi\sqrt{\pi}} \cdot \frac{1}{r^2} - \frac{3\sqrt{na}r_0^2}{4\pi\sqrt{\pi}} \cdot \frac{1}{r^4} + O\left(\frac{1}{r^6}\right) \quad (\text{B.5})$$

Which means that the asymptotic behavior $r \rightarrow \infty$ of $\rho(r)$ is one over distance squared¹. This behavior is correct at distances where the contribution from the second term in (B.5) can be neglected, i.e. $r \gg \sqrt{3/2} r_0 \approx r_0$ which means distances much larger than the healing length.

¹The $1/r^2$ dependence can be calculated directly from (1.45) by taking the limit $p \rightarrow 0$. Then $N_p \rightarrow mc/2p$ and integral (1.45) takes the form of a Fourier transform of a Coulomb potential $\int \exp(i\mathbf{k}\mathbf{r})/r \, d\mathbf{r} = 4\pi/k^2$ and produces the first term of eq. (B.5).

Acknowledgements

I would like to thank Prof. Sandro Stringari without whom this thesis would not exist. He gave me the opportunity to join his research group. Also I found invaluable his help in solving the organizational problems.

I would like to gratefully acknowledge the enthusiastic supervision of Dr. Stefano Giorgini and Prof. Lev P. Pitaevskii. They taught me so many new things and were always ready to answer any of my countless questions.

I would also like to thank Dr. Yuri E. Lozovik, my supervisor from Moscow Institute of Physics and Technology, who offered many insightful comments and suggestions and always supported me.

I am grateful to many people whom I meet in the University of Trento and who have assisted me so much in the course of this work.