CONTACT INTERACTIONS IN PATH INTEGRAL MONTE CARLO SIMULATIONS

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Chapter 1

Introduction

Physics is dead

- "There is nothing new to be discovered in physics now. All that remains is more and more precise measurement."- Lord Kelvin

- "It seems probable that most of the grand underlying principles have been firmly established. An eminent physicist remarked that the future truths of physical science are to be looked for in the sixth place of decimals."- Albert Michelson

These two sentences pronounced (presumably) by Kelvin and Michelson at late 19th century are, probably, among the most famous in history of science, yet also the most unfortunate ones. By that time, thermodynamics and electromagnetism had just been named, as well as mechanics was from earlier years, to be completed and perfectly well understood, but for some small patches that would be found with time and that would give more and more accurate predictions and explanations to measurements. Theoretical physics was dead, and it was time for experimentalists and engineers to rise and to take the control of science.

More than ever before

- "This spooky action at a distance."- Albert Einstein

It was not until a few years later that Plank, with his explanation of Black Body Radiation, founded quantum mechanics, a theory that would not start to be widely accepted until Einstein used it to explain the photoelectric effect. This way, these two long-lasting problems, that had given so many troubles and headaches to so many physicists during past decades, proved that not only physics was not dead, but that there was a whole new theory to be developed. Quantum physics was born, and a bunch of new possibilities, properties, answers and questions were brought to the game, making it amazing and funny to play again (possibly, more than ever before).

In the last hundred years, quantum theory has been much more developed and has shown a lot of interesting phenomena that are impossible to think about within a classical frame, and even it has lead to some technical applications. Nowadays, there is no doubt: quantum mechanics is the future. From quantum communications and teleportation of information to material science and nanoscale engineering, quantum world offers us an inimaginably large amount of possibilities, yet to be explored and understood.
Pen and paper

-"I think I can safely say that nobody understands quantum mechanics."- Richard Feynman

Quantum mechanics is well known for its strange (even weird) properties, and the difficulties to adress them theoretically and experimentally, due to its mathematical complexity and its extreme physical conditions such as size and temperature. Given these difficulties, and in order to (try to) understand this theory and its implications and consequences, physicists often make use of computer simulations.

In fact, nowadays it is almost impossible to think of research in any area of physics, chemistry or engineering without the help of computational techniques, and even more when dealing with quantum physics, where systems have so many degrees of freedom and are so complex to treat analytically. Actual research is not done with a pen and a paper: computers are the new laboratories.

1.1 Objectives and outline

This framework is where this present thesis is placed in. Our aim is to study the properties of one dimensional Bose gases where interatomic forces can be modeled by zero range interactions and at finite temperature, by means of a specific method for simulating quantum systems that has proven to be very effective: the "Path Integral Monte Carlo" method. To introduce this kind of potential in quantum simulations is not trivial and requires of a specific development.

Normally, the studies on this kind of systems are restricted to a single gas (sometimes with the addition of some impurities), while we are more interested in knowing what happens when dealing with full mixtures of two different gases. Therefore, we will focus on developing a code that is able to simulate this kind of systems, giving us freedom to tune proportion, mass and interaction strength of each one of the components.

This work follows this structure:

• Chapter 2: Theoretical basis. In this chapter we cover all most fundamental theoretical aspects related to the PIMC method. It can be split into two different fractions: first we focus on the basic theory needed to build up and to understand a simple PIMC code (sections one, two and three), and then we give a fast, not-too-in-deep description of possible ways to improve it (fourth section).

• Chapter 3: the Model. In this chapter we describe our specific model and how it has been implemented in our code.

• Chapter 4: Results. We present the results obtained with our PIMC code for different regimes, as could be systems at high and low temperatures, and with strong and weak interparticle interactions. We also contrast them with both experimental and theoretical results, when possible.
Chapter 2

Theoretical basis

In this chapter we want to discuss the theoretical aspects of this thesis, focussing on the Path Integral formalism and Monte Carlo simulations basics.

2.1 Monte Carlo methods and the Metropolis algorithm

Monte Carlo is a characteristic family of computational techniques in which approximations to solutions to quantitative problems are approached through stochastic sampling. This is, solving the problem by generating a set of suitable random numbers and observing the fraction of them obeying some property or statistical law (probability distribution).

The popularity of such algorithms has largely increased in the last decades since they can be used to solve problems and perform calculations that, given their large dimensionality, are very difficult (or even impossible) to solve with conventional methods in an acceptable amount of time. In addition, these problems can be of a very different nature, ranging from multi-dimensional numerical integration to the simulation of physical systems. For instance, the fact that such methods are based on random numbers imposes some uncertainty in their results, which make them very suitable for the simulation of quantum many-body and condensed matter’s randomly fluctuating systems, that are also characterized by a large amount of degrees of freedom.

An important concept in Monte Carlo simulations is the so called importance sampling. Let’s take an easy example in order to illustrate it: the computation of the expected value of some physical observable.

Let $O$ be a physical observable of a system composed of different states $\mu$ and its corresponding statistical weights $\omega_\mu (\sum_\mu \omega_\mu = 1)$. In a classical system at temperature $T$ the states are distributed according Boltzmann’s statistics: $\omega_\mu = Z^{-1} e^{-\beta E_\mu}$ and $Z = \sum_\mu e^{-\beta E_\mu}$. We define the average value of $O$ as:

$$\langle O \rangle = \sum_\mu \omega_\mu O_\mu$$

This sum must be performed over all possible states of the system (usually an infinite, or a very huge amount of them), so $\langle O \rangle$ can be computed analytically only in few cases. This way, we may want to sample $M$ states $\mu_i$ according to a probability distribution $p_\mu$ such that the truncated sum converges rapidly to the exact value, this is, to sample only those states that give an important contribution to the sum, while neglecting those that do not. In our example, the obvious choice would be to select $p_\mu = Z^{-1} e^{-\beta E_\mu}$, so the most contributing states would appear more frequently.

Hence the importance sampling defines the way sampled states are selected in order to the calculations to be more efficient, by using a probability distribution similar to the one that rules the simulated system.

2.1.1 The Metropolis algorithm

Now that we know how we should sample the system’s states in order to make the simulation more efficient, we may address the numerical method used to do so: the Metropolis algorithm.
The pseudo-random number generators commonly used in computer applications are able to sample uniformly the real numbers in the interval [0,1), but it is not trivial to use them in order to sample any probability distribution. With the Metropolis algorithm, one can efficiently perform this sampling by means of Markov Chains’ theory and stochastic processes, without worrying about the problem’s dimensionality nor the complexity of the desired probability distribution’s analytical form.

Basically, the algorithm bases the stochastic process’ time evolution in the following probability

\[ A(x_{i+1}|x_i) = \min \left( 1; \frac{p(x_{i+1})}{p(x_i)} \right) \]  

(2.2)

Where \( A(x_{i+1}|x_i) \) represents the probability of accepting the movement from configuration (state) \( x_i \) to \( x_{i+1} \), and \( p(x) \) the probability of the system to be in such state.

Therefore, the outline of the algorithm will be:

1. Given a state \( x_i \), compute the probability of the system to be in such configuration, \( p(x_i) \).
2. Using the pseudo-random number generator, propose a small movement towards a new configuration \( x' \) and compute the new probability, \( p(x') \).
3. Accept the trial with probability \( \alpha = A(x'|x_i) \). This is, if it is accepted, we make the system configuration change to \( x_{i+1} = x' \). Otherwise, the trial is rejected and \( x_{i+1} = x_i \).
4. Repeat the procedure as many times as wanted in order to generate the following system’s states. The final configuration will follow, asymptotically, the probability distribution \( p(x) \), plus a small random fluctuation.

### 2.2 The Path Integral Monte Carlo method

#### 2.2.1 Feynman’s Path Integral formalism

In order to compute the properties of a quantum system in thermal equilibrium, it is very useful (if not indispensable) to know its thermal density matrix \( \hat{\rho} \) [1], which can be written as:

\[ \hat{\rho} = Z^{-1} e^{-\beta \hat{H}} \]  

(2.3)

where \( \hat{H} \) is the Hamiltonian describing the system at temperature \( T \), \( \beta = (k_B T)^{-1} \) (\( k_B \) is the Boltzmann’s constant) and \( Z = Tr \left[ e^{-\beta \hat{H}} \right] \) is the partition function. Many properties we are interested in (the energy, the radial distribution function...) are diagonal in position space, so their expected value is given by:

\[ \langle \hat{O} \rangle = \int dR \rho(R; R; \beta) \hat{O}(R, R) \]  

(2.4)

With \( \rho(R_i, R_j; \beta) \) the thermal density matrix in space coordinate representation and \( R_i = \{ r_{1,i}, r_{2,i}, ..., r_{N,i} \} \) a particular set of the coordinates of the \( N \) particles of the system. In virtue of the convolution property eq. 2.5

\[ \rho(R_j, R_{j+2}; \beta_j + \beta_{j+1}) = \int dR_{j+1} \rho(R_j, R_{j+1}; \beta_j) \rho(R_{j+1}, R_{j+2}; \beta_{j+2}) \]  

(2.5)

we can rewrite the thermal density matrix as the convolution of \( M \) different paths:

\[ \rho(R_1, R_{M+1}; \beta) = \int dR_2...dR_M \rho(R_1, R_2; \tau) \rho(R_2, R_3; \tau) ... \rho(R_M, R_{M+1}; \tau) \]  

(2.6)

Therefore, by substitution of the thermal density matrix 2.6 in equation 2.4 the expression for computing the expected value of any physical observable in PIMC simulations reads

\[ \langle \hat{O} \rangle \simeq \int \prod_{j=1}^{M} dR_j \hat{O}(R_j) \rho(R_{i+1}, R_j; \tau) \]  

(2.7)
Where we have defined $\tau = \beta/M$, and with the boundary condition $R_{M+1} = R_1$ imposed by the trace.

Note that each density matrix, $\rho(R_j, R_{j+1}; \tau)$, in some sense, “connects” particle positions at time slice $j$ to the adjacent one at slice $j + 1$. Thus, we can think of the progression of particle positions from time slice to time slice as a discrete path. In a more formal way, we can see the thermal density matrix as an evolution operator in imaginary time $t = i\beta$, so equation 2.6 may be thought to describe an evolution in imaginary time from the initial configuration $R_1$ to the final one $R_{M+1}$ through a set of intermediate steps or “paths”.

This formalism, when applied to propagators in time, yields a new formulation of quantum mechanics where time evolution is computed with the exponential of the sum over all possible paths of the classical lagrangian of the system, where those paths closer to the classical one (the one that minimizes the action) appear with a higher probability.

### 2.2.2 The primitive approximation in PIMC simulations

Consider now a system of $N$ particles with mass $m$ interacting with a pair potential, described by a Hamiltonian $\hat{H} = \hat{K} + \hat{V}$, with $\hat{K}$ and $\hat{V}$ being the kinetic and the potential operators:

$$\hat{K} = -\frac{\hbar}{2m} \sum_{i=1}^{N} \nabla_i^2$$

$$\hat{V} = \sum_{i<j} v(r_i - r_j)$$

By direct substitution of this Hamiltonian in equation 2.3, we see that we may make use of the Baker-Campbell-Hausdorff formula to get an approximation for the thermal density matrix:

$$e^{-\tau(\hat{K}+\hat{V})} = e^{-\tau \hat{K}} e^{-\tau \hat{V}} e^{-\frac{\tau}{2} [\hat{K}, \hat{V}]} O (\tau^3)$$

So taking the limit of high temperature, or/and high number of paths, $\tau = \frac{\beta}{\tau} \to 0$ we can neglect terms of all higher than two orders in $\tau$, yielding the so called primitive approximation. This way, we write the thermal density matrix as

$$\rho = \frac{1}{Z} e^{-\tau \hat{K}} e^{-\tau \hat{V}}$$

In addition, it is important to point out that the kinetic and potential energy propagators can be explicitly calculated in the space of coordinates,

$$\langle R_{j+1} | e^{-\tau \hat{K}} | R_j \rangle = \left( \frac{2\pi \hbar^2}{m - \tau} \right)^{-\frac{D}{2}} e^{-\frac{m}{2\pi \tau} (R_{j+1} - R_j)^2}$$

$$\langle R_{j+1} | e^{-\tau \hat{V}} | R_j \rangle = e^{\tau V(R_j)} \delta (R_{j+1} - R_j)$$

Where $D$ is the dimensionality of the system, $\delta (R_{j+1} - R_j)$ is the Dirac’s delta distribution, $(R_{j+1} - R_j)^2 = \sum_{i=1}^{N} (r_{j+1}^{(i)} - r_j^{(i)})^2$ and $V(R_j) = \sum_{i,i'} v(r_{j+1}^{(i)} - r_j^{(i')})$, being both $i$ and $i'$ the particle’s indexes and $j$ the path’s one.

It must be noticed that, with this approximation, one is able to study systems at high temperatures (more classical) with a low number of paths, and at lower ones with a greater number of them. This fact gives an intuitive idea of how and why the lagrangian propagator works in the path integral formalism: in more classical systems (high $T$) particles are much likely to follow the classical action-minimizing path, hence we have to consider a fewer number of total possible paths, while in more quantum regimes the delocalization of particles is stronger, which is translated into a higher $M$.

This idea is also supported by the Trotter formula, which guarantees the convergence of the primitive approximation for high $M$:

$$e^{-\beta(\hat{K}+\hat{V})} = \lim_{M \to \infty} \left( e^{-\tau \hat{K}} e^{-\tau \hat{V}} \right)^M$$
As follows from the Trotter formula 2.14, the computation of \( \langle \hat{O} \rangle \) in the PIMC formalism eq. 2.7 (in our case, by means of the primitive approximation) is approximated for low \( M \), but becomes exact in the limit \( M \to \infty \). Hence, by increasing the number of paths in our simulations we are able to decrease the error made in the estimation of the expected value due to the approximation of the thermal density matrix, until the point that this approximative error is lower than the statistical one produced by the nature of the Monte Carlo method.

### 2.2.3 The pair product approximation

The primitive approximation gives us a good approach to the kinetic propagator. Nevertheless, the computation of the potential term can be more difficult, so we may use other approximations in order to take it into account. For our purpose, it results to be very useful the pair product approximation \([2]\)

\[
\rho (R, R'; \tau) \approx \left( \prod_{i=1}^{N} \rho_{sp}(r_j, r'_j; \tau) \right) \left( \prod_{i<j \in \mathcal{P}} \bar{\rho}_{rel}(r_{ii'}, r'_{ii'}; \tau) \right)
\]

(2.15)

where

\[
\rho_{sp}(r_i, r'_i; \tau) = \langle r_i | e^{-\tau H_{sp}^{\tau}} | r'_i \rangle
\]

(2.16)

is the single-particle density matrix and

\[
\bar{\rho}_{rel}(r_{ii'}, r'_{ii'}; \tau) = \frac{\rho_{rel}^{rel}(r_{ii'}, r'_{ii'}; \tau)}{\rho_{rel}^{rel}(r_{ii'}, r'_{ii'}; \tau_0)}
\]

(2.17)

denotes the normalized pair density matrix, being \( \rho_{rel}^{rel}(r_{ii'}, r'_{ii'}; \tau) = \langle r_{ii'} | e^{-\tau H_{rel}^{\tau}} | r'_{ii'} \rangle \) and \( \rho_{rel}^{rel}(r_{ii'}, r'_{ii'}; \tau_0) = \langle r_{ii'} | e^{-\tau H_{rel}^{\tau_0}} | r'_{ii'} \rangle \) the relative density matrices of the interacting and non-interacting two-body systems.

The key fact of the pair product approximation 2.15 is that the density matrices involved (one and two body density matrices, 2.16 and 2.17 respectively) can usually be calculated analytically. It is important to note that the pair product approximation does only account for single and two-body interactions, so three- and higher-body correlations do not apply. Hence, this approximation is only valid in the small \( \tau \) limit, so high temperature systems.

### 2.2.4 The classical isomorphism of PIMC

As we can see in equation 2.6, and as we have already discussed previously, each density matrix \( \rho(R_j, R_{j+1}; \tau) \), in some sense, "connects" particle positions at time slice \( j \) to the adjacent one at slice \( j + 1 \), but does not interact with these at positions \( j + 2 \) nor further away. This way, PIMC system of particles represented with a set of \( M \) different paths can be thought as a classical polymer \([15]\) of \( M \) beads, connected to their adjacent ones with a spring. Also, taking into account the boundary condition \( R_{M+1} = R_1 \) applied before, we note that these polymers form a closed ring. Hence, in the PIMC formalism quantum particles are mapped to a classical system of polymers with a number of harmonically coupled beads \( M \), which could be increased when dealing with lower temperatures.

With the expressions in 2.12 and 2.13, and using the primitive approximation, the final partition function of the system reads

\[
Z^{(p-a.)} = \int dR \rho^{(p-a.)}(R, R; \beta) = \left( \frac{2\pi \hbar^2}{m} \right)^{-\frac{DNM}{2}} \int dR_1 \cdots dR_M \exp \left[ -\sum_{i=1}^{M} \frac{m}{2\hbar^2 \tau} (R_{j+1} - R_j + 1)^2 + \tau V(R_j) \right]
\]

(2.18)

Which can be formally interpreted as a classical system with an effective hamiltonian

\[
H_{\text{eff}} = \sum_{i=1}^{M} \frac{m}{2\hbar^2 \tau} (R_{j+1} - R_j + 1)^2 + \tau V(R_j)
\]

(2.19)
Therefore we can use in principle all simulation techniques developed for classical systems to sample the path integral representation of the quantum system, by paying the prize of increasing the degrees of freedom of the problem from $DN$ (recall that $D$ is the dimensionality of the system considered) to $DNM$. Nevertheless, since Monte Carlo methods are designed for this specific multydimensional integrations, it is worth the price.

Figure 2.1: Classical isomorphism of a system of two quantum particles, each one represented by a polymer of five beads. Between particles, only beads with the same imaginary time index interact. Bead-bead interaction resembles that of a classical spring.

Sumarising, we have an effective classical hamiltonian that can be split in two terms, defining bead-bead in a single polymer and polymer-polymer interactions:

1. Bead-bead (intraparticle) interaction. The term $\sum_{i=1}^{M} \frac{m}{2\hbar^2} (R_{j+1} - R_{j+1})^2 = \frac{m}{2\hbar^2} \sum_{j=1}^{N} \sum_{j=1}^{M} (r_{j+1}^{(i)} - r_{j+1}^{(i)})^2$ can be regarded as harmonic springs acting between beads representing the same particle in successive imaginary time steps. The higher the temperature and the mass, the stronger become the springs, and so the polymer occupies a smaller volume, being the particle represented less delocalized (more classical).

2. Polymer-polymer (interparticle) interaction. The term $\sum_{i=1}^{M} \beta V(R_i) = \beta \sum_{i=1}^{M} \sum_{i,j'} v(r_{j+1}^{(i)} - r_{j+1}^{(i')})$ acts only between beads of different particles in the same imaginary time step, this is, in our notation, between beads with different index $i$ and same index $j$.

2.2.5 Simple case: 1D system with contact interactions in free space

In this thesis we focus in a simple system where we deal with a mixture of bose gases in one dimension, with contact interactions and in free space. In such a system the hamiltonian can be written as:

$$H^{rel} = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} + g\delta(x)$$  \hspace{1cm} (2.20)

and it can be shown that the normalized relative density matrix reads [3]
\[ \bar{\rho}^\text{rel}(x_j^{(i)}, x_j^{(i')}; \tau) = 1 - \frac{g}{\hbar} \sqrt{\frac{\pi \mu \tau}{2}} \exp \left[ -\mu \frac{x_j^{(i)} - x_j^{(i')}}{\tau \hbar^2} \right] \text{erfc}(u) \exp(u^2) \] (2.21)

where \( u = \sqrt{\frac{\pi \mu \tau}{\hbar^2}} \left| x_j^{(i)} + |x_j^{(i')}| + \tau \right| \) is the interaction strength in terms of the 1D effective scattering length \( a_{1D} \) \[9\] \[10\].

Using the primitive approximation, and being the hamiltonian of a single particle \( H^{sp} = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} \), the single particle density matrix is \[4\]

\[ \rho^{sp}(x_j^{(i)}, x_j^{(i')}; \tau) = \left( \frac{\mu}{2\pi \tau \hbar^2} \right)^{1/2} \exp \left[ -\mu \frac{(x_j^{(i)} - x_j^{(i')})^2}{2\tau \hbar^2} \right] \] (2.22)

We will study the system by directly applying the pair product approximation to these equations and by means of a PIMC code.

### 2.3 Computation of the system’s properties

In the section The Path Integral Monte Carlo method we have discussed how to compute the expected value of some properties in the Feynman’s path integral formalism of quantum mechanics. The path-integral mapping allows us to easily calculate the average of any operator which is diagonal in the position representation eq. 2.7.

Nevertheless, there are some interesting system’s properties as the total energy per particle that are not diagonal in this representation, so computing it in this way would not be trivial.

#### 2.3.1 Radial distribution function

The radial distribution function (or RDF) is an example of a pair correlation function, which describes how, on average, the atoms in a system are radially (in the general three-dimensional case) packed around each other. This proves to be a particularly effective way of describing the average structure of disordered systems, and, since it can be easily measured experimentally by means of x-ray or neutron diffraction studies, it is a very powerful way to provide a direct comparison between experiments and simulations.

The estimator for the RDF is \[5\]

\[ g(r) = \langle n(r) \rangle = \frac{V}{N^2 M} \sum_{j=1}^{M} \sum_{i \neq i'} \delta \left( r - \left( r_j^{(i)} - r_j^{(i')} \right) \right) \] (2.23)

Where \( \frac{V}{N^2} \) is a normalization constant and we have considered, in addition, an average over the bead indexes since, due to the symmetry over imaginary time paths, all the configurations \( R_j \), with \( 1 \leq j \leq M \), can be considered in the evaluation of the RDF to take advantage of larger statistics.

In order to estimate the expectation value of the \( \delta \) function in equation 2.23, we construct an histogram where we compute the frequencies of appearance of the relative distances between beads of different particles and same bead indexes.

#### 2.3.2 Total energy per particle

One of the most important properties we’d like to compute is the total energy per particle, and it turns out that it is easier to derive the classical thermodynamic estimator from the partition function than to apply equation 2.7.

\[ \frac{E}{N} = -\frac{1}{N \beta} \frac{\partial Z}{\partial \beta} \] (2.24)
In a similar way to eq. 2.18, for a bosonic system in one dimension we can write the partition function in the PIMC formalism as

\[
Z = \frac{1}{N!} \sum_{\rho} \prod_{j=1}^{M} dR_j \left( \frac{2\pi\hbar^2}{m} \right)^{-\frac{N}{2}} \exp \left[ -S \left( R_{j+1}, R_j; \tau \right) \right]
\]

(2.25)

With \( S \) the action of the system:

\[
S \left( R_{j+1}, R_j; \tau \right) = -\ln \left[ \rho \left( R_{j+1}, R_j; \tau \right) \right] = \frac{1}{4\lambda \tau} \left( R_{j+1} - R_j \right)^2 + U \left( R_{j+1}, R_j; \tau \right)
\]

(2.26)

Where we have defined \( \lambda = \frac{\hbar^2}{2m} \). By directly applying the equation 3.5 to the partition function in 2.25 we obtain the thermodynamic estimator for the total energy per particle:

\[
\frac{E_T}{N} = \left\langle \frac{1}{2\tau} - \frac{1}{MN} \sum_{j=1}^{M} \left( x_j^{(i)} - x_{j+1}^{(i)} \right)^2 + \frac{1}{MN} \sum_{j=1}^{M} \frac{\partial U \left( x_j^{(i)}, x_{j+1}^{(i)}; \tau \right)}{\partial \tau} \right\rangle
\]

(2.27)

Note that the first term is \( M \) times the energy of a classical ideal gas.

Clearly, the sum of both the first and second terms of this expression correspond to the kinetic energy. At first look it might look strange because of the negative sign in front of the energy of the springs, meaning that the faster the particle moves along the path between slices \( j \) and \( j+1 \), the lower the kinetic energy will be. This paradox is resolved when one realizes that we are dealing with imaginary time path integral, so the sign is reverted. In fact, it is consistent with the uncertainty principle: the more delocalized the particle is, the lower the kinetic energy: when the particle is confined to stay within a small region of space, the kinetic energy is large.

From the approximation to the density matrix used and the definition of the action and equation 3.5 it follows that:

\[
U \left( x_j^{(i)}, x_{j+1}^{(i)}; \tau \right) = \prod_{i} \rho_i \left( x_j^{(i)}, x_{j+1}^{(i)}; \tau \right)
\]

(2.28)

So, taking its derivative with respect to \( \tau \), one finally gets an analytical expression for the thermodynamic estimator:

\[
\frac{\partial U \left( x_j^{(i)}, x_{j+1}^{(i)}; \tau \right)}{\partial \tau} = e^{\sum_i \ln \rho_i} \sum_i \frac{\partial \ln \rho_i}{\partial \tau}
\]

(2.29)

With

\[
\rho_i \left( x_j^{(i)}, x_{j+1}^{(i)}; \tau \right) = \left[ 1 - g \frac{\pi \mu \tau}{2} \exp \left( -\mu \frac{x_j^{(i)} x_{j+1}^{(i)} + x_j^{(i)} x_{j+1}^{(i)} \langle \tau \rangle}{\tau \hbar^2} \right) \right] \exp \left( u^2 \right)
\]

(2.30)

and the derivative of its logarithm:

\[
\frac{\partial \ln \rho \left( x_j^{(i)}, x_{j+1}^{(i)}; \tau \right)}{\partial \tau} = g \frac{\pi \mu}{2} \frac{\mu}{\hbar^2} \frac{1}{\tau \hbar^2} f(u) + \frac{1}{2\pi \tau^2} f(u) - \mu \frac{x_j^{(i)} x_{j+1}^{(i)} \langle \tau \rangle}{\tau \hbar^2} \left[ 2uf(u) - \frac{u^2}{2} \right]
\]

(2.31)

Where we have defined \( f(u) = erfc(u) \exp \left( u^2 \right) \).
A small numerical problem: $erfc(u)$ versus $exp(u^2)$

An important part of the interparticle forces computation relies on the term $f(u) = erfc(u) exp(u^2)$.

Since we must deal with a very large number, corresponding to the exponential, and a very small one corresponding to the complementary error function of a positive number (we can see that $u$ is always larger than 0, since we are only interested in positive values of $g$) the computation of this term is not a problem straightforward to adress numerically.

![Figure 2.2: $exp(u^2)$ versus $erfc(u)$ in a logarithmic scale](image)

We can solve this problem by knowing that $erfc(u)$ is always bounded, for positive values of $u$, by the following functions [6]

$$
\frac{2exp(-u^2)}{\sqrt{\pi}(u + \sqrt{u^2 + 4})} < erfc(u) \leq \frac{2exp(-u^2)}{\sqrt{\pi}(u + \sqrt{u^2 + 4})}
$$

(2.32)

![Figure 2.3: Comparision of $erfc(u)$ and its upper and lower bounds](image)

So we decide to take the upper bound as a good approximation for $erfc(u)$. Then, by inspection
of the upper bound formula, we decide to implement into the code the full term as

$$erfc(u) \exp(u^2) \approx \frac{2}{\sqrt{\pi}} \left( u + \sqrt{u^2 + \frac{1}{4}} \right)$$

(2.33)

which is a very accurate approximation as we can see in the figure below fig.2.4, where we plot the absolute error in a logarithmic scale.

![Absolute error of the approximation](image)

Figure 2.4: Absolute error of the approximation

### 2.4 Higher order approximations and improvements

Until now, we have presented all the theory that we will need and use in order to simulate physical systems in this thesis. Nevertheless, there are some improvements that could be taken into account if we’d like to look closer and with smaller errors to some properties.

In this section we want to take some not too in depth look at these possible improvements to our method.

#### 2.4.1 Better approximations of the action

The only approximation to the action considered in previous sections, along with the pair-product, is the primitive approximation. As we have already discussed, this rough approximation is the simplest way to approach the thermal density matrix at high temperatures. However, it presents the disadvantage that, for lower temperatures, the number of beads needed in order to the method to give some feasible results keeps increasing, making the convergence of this approximation to the exact density matrix particularly slow for a high number of particles.

Hence, the primitive approximation gives us a good approach to the study of semiclassical systems, where the quantum effects are relatively small. If we were interested in highly correlated systems like the ones presenting, for example, Bose-Einstein condensation or superfluidity of liquid helium, it would be imprescindible to work with higher order, more complex approximations of the action that allowed us to explore these more quantum and much more interesting regimes.
The Takahashi-Imada approximation

The most obvious and simplest, better approximation to the action than the primitive one consists in taking a larger order expansion of the propagator $e^{-\tau \hat{H}}$ from the Baker-Campbell-Hausdorff formula 2.10. This is, in the same way we derivated the primitive approximation, truncate the series expansion at a higher order in $\tau$ [17] [18], taking

$$e^{-\tau (\hat{K}+\hat{V})} \approx e^{-\tau \hat{K}} e^{-\tau \hat{V}} e^{-\frac{\tau^2}{12!}[[[\hat{V},\hat{K}],\hat{V}]]}$$ (2.34)

instead of

$$e^{-\tau (\hat{K}+\hat{V})} \approx e^{-\tau \hat{K}} e^{-\tau \hat{V}}$$ (2.35)

as we did in the primitive approximation.

An important advantage of the Takahashi-Imada approximation 2.34 in front of the primitive one 2.35 is that we are able to improve the approximation for the trace (which is the important point if we want to compute thermodynamic properties) up to $\tau^4$, with the only addition of the term containing the double commutator $[[[\hat{V},\hat{K}],\hat{V}]]$, which is relatively easy to evaluate:

$$[[[\hat{V},\hat{K}],\hat{V}]] = \hbar^2 \frac{m}{|\nabla V|^2}$$ (2.36)

and, since it only depends on the gradient of the potential, we can usually compute it without too many problems.

For practical purposes, a PIMC simulation with Takahashi-Imada approximation is equivalent to a simulation with the primitive approximation where, in the potential propagator in equation 2.13, we substitute $V (r)$ with the term:

$$W (R) = \sum_{i,i'} v \left( r_{j+1}^{(i)} - r_{j+1}^{(i')} \right) + \frac{\tau^2 \hbar^2}{24m} \sum_{i=1}^{N} \sum_{i' \neq i} \left| \nabla_i v \left( r_{j+1}^{(i)} - r_{j+1}^{(i')} \right) \right|^2$$ (2.37)

The Chin approximation

The next better way to compute the action with more accuracy would be to consider a symplectic expansion of the Takahashi-Imada approximation. This is to consider an expansion of the form:

$$e^{\tau (\hat{K}+\hat{V})} = \prod_l e^{-\alpha_l \tau \hat{K}} e^{-\gamma_l \tau \hat{V}} e^{-\omega_l \tau [[[\hat{V},\hat{K}],\hat{V}]}}$$ (2.38)

and to find a set of coefficients $\alpha_l, \gamma_l, \omega_l$ which make this symplectic expansion a good approximation for the action up to sixth order in $\tau$.

In the Chin approximation, this factorization is given by:

$$e^{-\tau \hat{H}} \approx e^{-\gamma_1 \tau \hat{W}_{a_1}} e^{-\alpha_1 \tau \hat{K}} e^{-\gamma_2 \tau \hat{W}_{a_2}} e^{-\alpha_1 \tau \hat{K}} e^{-\gamma_1 \tau \hat{W}_{a_1}} e^{-2\alpha_0 \tau \hat{K}}$$ (2.39)

where

$$\hat{W}_{a_l} = \hat{V} + \frac{u_0}{\nu_l} \alpha_l^2 \left( [[[\hat{V},\hat{K}],\hat{V}]] \right)$$ (2.40)

And where the parameters in equations 2.39 and 2.40 must satisfy [5]

$$u_0 = \frac{1}{12} \left[ 1 - \frac{1}{1 - 2\alpha_0} + \frac{1}{6(1 - 2\alpha_0)^3} \right]$$ (2.41)

$$\gamma_1 = \frac{1}{6(1 - 2\alpha_0)^2}$$ (2.42)

$$\gamma_2 = 1 - 2\gamma_1$$ (2.43)

$$\alpha_2 = 1 - 2\alpha_1$$ (2.44)
\[ \alpha_1 = \frac{1}{2} - \alpha_2 \]  
\[ 0 \leq \alpha_1 \leq 1 \] (2.45)  
\[ 0 \leq \alpha_1 \leq \frac{1}{2} \left( 1 - \frac{1}{\sqrt{3}} \right) \] (2.46)  
\[ 0 \leq \alpha_1 \leq 1 \] (2.47)

The accuracy of the Chin Approximation depends on the particular values of \( \alpha_1 \) and \( \alpha_0 \), that have to be optimized. The optimal values are those achieving an approximate cancelation of the various high-order commutators in the leading fourth-order error. These optimal values are, therefore, independent of the temperature and they can be easily determined numerically carrying out simulations at high temperatures.

**The permutation sampling**

Until now, we have assumed the particles we are working with to be distinguishable. The problem is that, when we want to work with many-body systems at very low temperatures, quantum correlations and effects are stronger and the statistics of particles cannot be neglected. In order to take it into account, a good PIMC code must include what is called *Permutation sampling*.

Basically, the permutation sampling can be implemented by assuming not always closed rings, but polymers that can, instead, open, close, swap conformation, and even make bigger rings by coupling two chains. Nevertheless, due to the complexity of this permutation, we do not cover it in this thesis.

### 2.4.2 Other interesting properties

In this thesis we have focused on the study of the properties of bose gasses by means of the computation of the total energy per particle and the radial distribution function. Nevertheless, there are other interesting properties that can be computed and that could give us more information about our system.

**Potential and kinetic energies**

We have already seen in detail how to compute the total energy per particle. However, sometimes we may be more interested in estimating only the kinetic or the potential energies, instead of the total sum.

As we have seen, when using the primitive approximation, it is a trivial problem because we can easily distinguish the two components of the energy in the total energy estimator: since the third term \( U \) does not depend on the mass of the particle, kinetic and potential energies are not coupled and they can be identified with the sum of the two first terms for the kinetic contribution and the third one for the potential (see equation 2.27). Nevertheless, for higher order approximations this direct identification is not possible and hence we have to compute these contributions with a different estimator.

For instance, we can compute the kinetic energy in a similar way to the one used for the total energy, by means of a thermodynamic estimator:

\[ \frac{K}{N} = -\frac{m}{\beta Z} \frac{dZ}{dm} \] (2.48)

Which, for the partition function eq. 2.25 gives the following expression for the computation of the kinetic contribution:

\[ \frac{E_T}{N} = \left( \frac{1}{2\tau} - \frac{1}{MN} \sum_{j=1}^{M} \left( x_{j}^{(i)} - x_{j+1}^{(i)} \right)^2 \right) + \frac{m}{MN\tau} \sum_{j=1}^{M} \frac{\partial U \left( x_{j}^{(i)}, x_{j}^{(i)'}; \tau \right)}{\partial m} \] (2.49)

In order to estimate the potential energy we can make use of the simple relation \( E_T = K + V \), being \( E_T, K \) and \( V \) the total, kinetic, and potential energies, respectively. Hence the estimator for the potential energy reads:
\[
\frac{V}{N} = \left\langle \frac{1}{MN} \sum_{j=1}^{M} \left( \frac{\partial U(x_j^{(i)}, x_j^{(i)}; \tau)}{\partial \tau} - \frac{m}{\tau} \frac{\partial U(x_j^{(i)}, x_j^{(i)}; \tau)}{\partial m} \right) \right\rangle \tag{2.50}
\]

Being \( U \) a function dependent on the approximation used.

**A better approach to the total energy per particle**

As we can see in the thermodynamic estimator for the total energy eq. 2.27, for low values of \( \tau \) (which are needed in order to do the simulations correctly) the first and second terms of the equation are large, making the computation of their difference very difficult to perform and hence the estimation of the total energy very imprecise.

In order to overcome this problem, there is the possibility of using the so called **Virial estimator** for the total energy [20]:

\[
\frac{E_V}{N} = \frac{1}{2\beta} + S_1 + S_2 + S_3 \tag{2.51}
\]

Where

\[
S_1 = \left\langle \frac{1}{N} \sum_{j=1}^{M} \left( x_M^{(i)} - x_j^{(i)} \right) \left( x_M^{(i+1)} - x_M^{(i)} \right) + \right\rangle \tag{2.52}
\]

\[
S_2 = \left\langle \frac{1}{2\beta N} \sum_{j=1}^{M} \left( x_j^{(i)} - \bar{x}_j^{(i)} \right) \frac{\partial}{\partial x_j^{(i)}} \left[ U \left( x_j^{(i)}, x_j^{(i)}; \tau \right) + U \left( x_j^{(i+1)}, x_j^{(i+1)}; \tau \right) \right] \right\rangle \tag{2.53}
\]

\[
S_3 = \left\langle \frac{1}{MN} \sum_{j=1}^{M} \frac{\partial U(x_j^{(i)}, x_j^{(i)}; \tau)}{\partial \tau} \right\rangle \tag{2.54}
\]

In equation 2.53 we have defined \( \bar{x}_j^{(i)} = \frac{1}{2M} \sum_{j' =1}^{M-1} \left( x_j^{(i)} + x_j^{(i)} \right) \).

**Static structure factor**

We have already discussed how we can compute the radial distribution function in order to study the spatial configuration of atoms. Nevertheless, often times this information is not enough to completely characterize our system, and we may also want to infer into the order of atoms in the reciprocal space. To do so, we can compute the so called **Static structure factor** \( S \), defined as:

\[
S(q) = \frac{1}{NZ} \int dR \rho(R, R; \beta) \left( \sum_{i=1}^{N} e^{-iqr^{(i)}} \right) \left( \sum_{i'=1}^{N} e^{-iqr^{(i')}} \right) \tag{2.55}
\]

Since we deal with periodic boundary conditions and with a system restricted to one single dimensional box of size \( L \), the wave vector \( q \) reads:

\[
q = 2\pi \frac{n}{L} \tag{2.56}
\]

with \( n \) an integer number.

Then, the estimator for the static structure factor is given by

\[
S(q) = \frac{1}{NM} \left\langle \sum_{i \neq j}^{M} \left[ \cos \left( qx_j^{(i)} \right) \cos \left( qx_j^{(i')} \right) + \sin \left( qx_j^{(i)} \right) \sin \left( qx_j^{(i')} \right) \right] \right\rangle \tag{2.57}
\]

Note that, similarly as we did when computing the radial distribution function, we could sum only for a single bead index, but we take the average over all imaginary times so we can have the advantage of larger statistics.
Further away: quantum properties

One would think now about how to read, from the already discussed properties, quantum regimes such as Bose-Einstein condensation or superfluidity. In fact, for doing so we should compute other properties, for instance the One Body Density Matrix (OBDM) or the Superfluid Density, and explore their behaviour under certain circumstances. Nevertheless, the computation of these properties demands a complex PIMC method including the permutation sampling, and so we will not cover it in this thesis.
Chapter 3

The model

As we have already said before, in this thesis we focus on the study of one-dimensional Bose gases with contact interactions, by means of the development of a PIMC method code. The principal purpose was to construct a code as general as possible, that was able to work with full mixtures (instead of just impurities) of two different Bose gases, with different mass and even with different contact interaction strengths (nevertheless, following the assumption needed to make the necessary approximation in eq. 2.32, we have constrained the contact interactions to be repulsive).

Recalling the primitive- and pair-product- approximations, we base our Monte Carlo sampling in the following equations [4]:

\[
\rho(R, R'; \tau) \approx \left( \prod_{j=1}^{N} \rho^{sp}(r_j, r_j'; \tau) \right) \left( \prod_{i<j} \rho^{rel}(r_{ii'}, r_{ii'}'; \tau) \right) \tag{3.1}
\]

\[
\rho^{rel}(x_j^{(i)}, x_{j'}^{(i')}; \tau) = 1 - \frac{g}{\hbar} \sqrt{\frac{\pi \mu \tau}{2}} e^{\frac{\mu}{\hbar^2} \left( |x_j^{(i)}| + |x_{j'}^{(i')}| - g \tau \right)} \text{erfc} \left( \frac{u}{\hbar} \right) \exp \left( u^2 \right) \tag{3.2}
\]

\[
\rho^{sp}(x_j^{(i)}, x_{j+1}^{(i)}; \tau) = \left( \frac{\mu}{2\pi \tau \hbar^2} \right)^{\frac{1}{2}} e^{\frac{\mu}{\hbar^2} \left( x_j^{(i)} - x_{j+1}^{(i)} \right)^2} \tag{3.3}
\]

Where we use \( j \) to denote bead index and \( i, i' \) different particle indexes. In equation 3.2 \( u = \sqrt{\frac{\pi}{2\tau \hbar^2}} \left( |x_j^{(i)}| + |x_{j'}^{(i')}| + g \tau \right) \).

In this section we are going to address how this model has been implemented in our code, as well as the computation of the properties of the system.

3.1 Variables and parameters

We first want to describe the variables involved in the code so that it is easier for the reader to understand how it works. There are, basically, four different kinds of variables: system parameters, physical constants, inner-code variables and data storing variables. We are going to describe each kind of variable separately.

3.1.1 System parameters

System parameters are these variables introduced in the beginning of the code in order to control the basic initial properties of the system that we want to simulate, such as the boxlength or the mass of the particles. Since they play such an important role in the code, we may address them one by one.

\( N_{\text{links}} \) is the number of "paths" considered in the path integral formalism, or the number of beads used to build the polymers.
L is the boxlength.
N_mov is the number of time steps that the simulation will last for.
N_hist is the number of bins used to compute the radial distribution function’s histogram.
\( \rho_A \) and \( \rho_B \) are the initial number densities of each kind of particles.
\( M_A \) and \( M_B \) are the masses of each kind of particles.
\( T_0 \) is the initial temperature of the system.
\( g_A, g_B \) and \( g_{AB} \) are the strengths of the different interparticle interactions, between two particles of the spice A, two particles of the spice B, or two particles of different spices, respectively.
\( c_{dx_{bb}} \) is the maximum range of length of the proposed bead-bead movement in the Monte Carlo sampling. If \( c_{dx_{bb}}=1 \), for example, then the proposed bead-bead movements will range between \(-0.5\) and \(+0.5\).
\( c_{dx_{cm}} \) is the same as \( c_{dx_{bb}} \), but corresponding to the center of mass movements.
\( bb_{rat} \) is the ratio between the number of bead-bead and center of mass movements. Since bead-bead movements are much faster to sample, one may want \( bb_{rat} \) to be higher than 0.5, but not too high since it would not represent a realistic simulation.

### 3.1.2 Physical constants

Only two physical constants are needed for the simulations we are interested in: Boltzmann’s constant \( k_B \), named \( Kb \) in the code, and Plank’s reduced constant, \( \hbar \) (\( hb \) in the code). For convenicene, we set both their values to \( k_B = 1 \) and \( \hbar = 1 \).

In this section we also introduce useful mathematical constants such as \( \pi \), named \( pi \), and \( \sqrt{\pi} \), \( spi \).

### 3.1.3 Inner-code variables

There are a bunch of variables that need to be declared in order to the code to work properly. Nevertheless, most of them do not play an important role and naming them during the explanation of further parts of the code will be enough for the reader to understand how they work.

### 3.1.4 Data storing variables

Data storing variables are these matrices and vectors where data of different properties of the system is stored. By taking a look at them we are able to plot the time evolution of some properties and to make some conclusions from the simulations.

RDF stores the computed radial distribution function, and the matrix FS the position of every single bead of all particles of the system, aswell as the mass of each particle and wether it is A or B type.

Every column of FS represents a different particle. The last two numbers indicate its mass and its type (\( lastnumber = 0 \) for A particles, and \( lastnumber = 1 \) for B ones), and the other ones each bead’s position. In figure 3.2, for example, we can see seven different particles, two of them of type B (with mass \( m_B = 2 \)) and five of type A (\( m_A = 1 \)).

### 3.2 Initial configuration

Before starting the simulation, it is important to set some variables to its propper value. This is the case for the acceptance rates acc_bb (acceptance rate of bead-bead movements) and acc_cm.
3.2 Movement of particles

As we have already seen, we consider two basic types of movement during the simulation: bead-bead and center of mass. Every time step the type of movement that will be carried out is chosen randomly (although we can tune its approximate rate with the initial variable \( \text{bb\_rat} \), just as we have seen in past sections). In order to choose it, we call a random number in the variable \( \text{bb\_cm} \) that ranges between 0 and 1, and compare it with \( \text{bb\_rat} \): if the random number is below this value, the movement chosen will be bead-bead, and center of mass if it is larger. We also have to choose randomly a particle to move.

We also have to make sure that, when running over the bead indexes, \( n_b \), the polymers are closed chains, see figure fig.3.5.

3.3 Movement of particles

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We also have to make sure that, when running over the bead indexes, \( n_b \), the polymers are closed chains, see figure fig.3.5.
3.3.1 Bead-bead movement

Bead-bead movement consists in proposing a small variation in the position of each bead of the particle selected. So running the index \(i_b\) from the first bead of the particle to the last one, we have to sample for each bead the density matrix term corresponding to a single particle and the one corresponding to the interparticle forces.

Let’s first adress the single particle sampling eq.3.3. For each bead, the single particle density matrix depends on the exponential of the relative distance between it and the following one.

In order to sample the single particle density matrix, we compute the values \(x_{rel}\) and \(y_{rel}\), that represent the distance from the bead that is being sampled to the next and the precessing ones, all of them of the same particle. Then we apply the corresponding equation and we store this value in the variable \(V_o\) (“V old”).

We propose a small movement for the chosen bead and compute its new value, which we store in the variable \(V_n\) (“V new”).

We may now adress the computation of the two-body density matrix terms eq.3.2 (both old and new values), which will multiply, in virtue of the pair product approximation eq.3.1 the already computed \(V_o\) and \(V_n\) variables.

Note that expression 3.2 accounts for the two body interaction for up to second order, this is, we may compute not only the relative distance between bead \(j\) of the selected particle and bead \(j\) of all other particles, but also the same for beads \(j - 1\) and \(j + 1\). In the code’s notation, distance

! select randomly the type of movement
\[
\text{call random_number(bb_cm)}
\]

! select randomly a particle to move
\[
\text{call random_number(nn)}
\]
\[
n=\text{int}(\text{nn}*\text{N_part})+1
\]

Figure 3.4: Random selection of the movement

\[
do\ i_b=1,\text{N_links}
\]
\[
! \text{closed chains}
\]
\[
i_{\text{cm}1}=i_b-1
\]
\[
i_{\text{bp}1}=i_b+1
\]
\[
\text{if } (i_b,\text{eq.1}) \text{ then}
\]
\[
i_{\text{km}1}=\text{N_links}
\]
\[
\text{end if}
\]
\[
\text{if } (i_b,\text{eq.N_links}) \text{ then}
\]
\[
i_{\text{bp}1}=1
\]
\[
\text{end if}
\]

Figure 3.5: Make sure that the polymer is a closed chain

\[
\text{3.3.1 Bead-bead movement}
\]

\[
\text{Bead-bead movement consists in proposing a small variation in the position of each bead of the particle selected. So running the index } i_b \text{ from the first bead of the particle to the last one, we have to sample for each bead the density matrix term corresponding to a single particle and the one corresponding to the interparticle forces.}
\]

\[
\text{Let’s first adress the single particle sampling eq.3.3. For each bead, the single particle density matrix depends on the exponential of the relative distance between it and the following one.}
\]

\[
\text{In order to sample the single particle density matrix, we compute the values } x_{rel} \text{ and } y_{rel}, \text{ that represent the distance from the bead that is being sampled to the next and the precessing ones, all of them of the same particle. Then we apply the corresponding equation and we store this value in the variable } V_o \text{ (“V old”).}
\]

\[
! \text{single particle interaction}
\]
\[
x_{rel} = \text{FS}(i_b,n) - \text{FS}(i_{bp1},n)
\]
\[
y_{rel} = \text{FS}(i_b,n) - \text{FS}(i_{km1},n)
\]
\[
\text{if } (\text{abs}(x_{rel}) > (1/2)) \text{ then}
\]
\[
x_{rel} = x_{rel} - \text{sign}(1.0*1,x_{rel})
\]
\[
\text{end if}
\]
\[
\text{if } (\text{abs}(y_{rel}) > (1/2)) \text{ then}
\]
\[
y_{rel} = y_{rel} - \text{sign}(1.0*1,y_{rel})
\]
\[
\text{end if}
\]
\[
V_o = -c*\text{FS}(x_{rel}**2+y_{rel}**2)
\]

Figure 3.6: Boundary conditions and computation of \(\rho_{D,free}^{rel,0}(x,x';\tau)\)

We propose a small movement for the chosen bead and compute its new value, which we store in the variable \(V_n\) (“V new”).

We may now adress the computation of the two-body density matrix terms eq.3.2 (both old and new values), which will multiply, in virtue of the pair product approximation eq.3.1 the already computed \(V_o\) and \(V_n\) variables.

Note that expression 3.2 accounts for the two body interaction for up to second order, this is, we may compute not only the relative distance between bead \(j\) of the selected particle and bead \(j\) of all other particles, but also the same for beads \(j - 1\) and \(j + 1\). In the code’s notation, distance
between beads of index \( j \) is called \( x_{\text{rel}} \), and for beads \( j-1 \) and \( j+1 \) variables \( y_{\text{rel}} \) and \( y_{\text{prel}} \) are used, respectively. See figure fig.3.7.

```plaintext
! interparticle distances
x_{\text{rel}}=F(i_{\_b},n)-F(i_{\_b},i_{\_n})
y_{\text{rel}}=F(i_{\_b},1,n)-F(i_{\_b},1,n)
y_{\text{prel}}=F(i_{\_b},1,n)-F(i_{\_b},1,n)
if (abs(x_{\text{rel}})<(L/2)) then
  x_{\text{rel}}=x_{\text{rel}}-sign(1.0*L,x_{\text{rel}})
end if
if (abs(y_{\text{rel}})<(L/2)) then
  y_{\text{rel}}=y_{\text{rel}}-sign(1.0*L,y_{\text{rel}})
end if
if (abs(y_{\text{prel}})<(L/2)) then
  y_{\text{prel}}=y_{\text{prel}}-sign(1.0*L,y_{\text{prel}})
end if
```

Figure 3.7: Computation of interparticle distances

Here we also have to compute the reduced mass \( \mu \), called \( M_r \) in the code and the corresponding interaction strength (named \( g_{\text{int}} \)), depending whether the interaction is between two \( A \) particles, two \( B \) particles, or one of each type.

We compute the interparticle force term and multiply it with the already computed free particle one, in virtue of the pair-product approximation, see figure 3.8.

```plaintext
up=Mr*(abs(x_{\text{rel}})+abs(y_{\text{prel}})+g_{\_A*tau})
  / (sqrt(2*Mr*tau*hb**2))
  fup=2/(spi*(up+sqrt((up**2+4/pi)))
  mum=Mr*(abs(x_{\text{rel}})+abs(y_{\text{rel}})+g_{\_A*tau})
  / (sqrt(2*Mr*tau*hb**2))
  fum=2/(spi*(um+sqrt((um**2+4/pi)))

Vo=exp(-Mr*[x_{\text{rel}}*y_{\text{prel}}+abs(x_{\text{rel}}*y_{\text{prel}})]
  / (tau*hb**2))
Vom=exp(-Mr*[x_{\text{rel}}*y_{\text{rel}}+abs(x_{\text{rel}}*y_{\text{rel}})]
  / (tau*hb**2))
V=Vo*[1-Vo*xfu*fup]*[1-Vo*xfu*fum]
```

Figure 3.8: Pair-product approximation: \( Vo=Vo*(\text{interparticle terms}) \)

Again, we propose a small movement (exactly the same one proposed when computing the single particle contribution) for the chosen bead and compute its new value, which we store in the variable \( V_n \).

After having taken into account all interparticle interactions, we have the final values of \( V_o \) and \( V_n \), which we have to compare in order to choose whether the proposed movement is accepted or not, with the corresponding probability given by the Metropolis algorithm eq.3.4:

\[
A(x_{i+1}|x_i) = \min \left( 1, \frac{p(x_{i+1})}{p(x_i)} \right)
\]  

(3.4)

Note that, when the movement is accepted, we have to check that the new position of the bead is within the boxlength, and apply the periodic boundary conditions if it lies outside of it.

### 3.3.2 Center of mass movement

Center of mass movement consists in proposing a small variation in the position of the whole selected particle, this is, the same variation for the position of all of its beads. It is basically
computed in the same way as the bead-bead movement, so we will not extend this section as much as the bead-bead one.

First we have to notice that, since every bead of the particle is moving equally, their relative position with each other will not change, so we can exclude the computation of the single particle density matrix.

Nevertheless, we have to compute, for every single bead of the moving particle, the two body action with respect to all other particles, which makes this kind of movement much slower to sample (assuming that a large enough number of beads is used for the simulation). This fact may make us want to tune the ratio between the number of bead-bead and center of mass movements (remember that the type of movement is selected randomly with a given probability), by changing the value of the variable $bb_{\text{rat}}$ as we have already explained in past sections.

In a center of mass movement, it is important to move every single bead of the particle, once the movement has been accepted, so the metropolis and the boundary conditions routines must be slightly changed.

```fortran
! Metropolis
if (Vn.le.Vo) then
   do i_b=1,N_links
      FS(i_b,n)=FS(i_b,n)+dx
   enddo
   acc_cm=acc_cm+1
else
   call random_number(r)
   mov=exp(-beta*(Vn-Vo))
   if (r.lt.mov) then
      do i_b=1,N_links
         FS(i_b,n)=FS(i_b,n)+dx
      enddo
      acc_cm=acc_cm+1
   endif
endif

! Boundary conditions
do i_b=1,N_links
   if (FS(i_b,n)>L) then
      FS(i_b,n)=FS(i_b,n)-L
   endif
   if (FS(i_b,n)<-L) then
      FS(i_b,n)=FS(i_b,n)+L
   endif
enddo
```

Figure 3.9: Accept or reject the proposed movement following the Metropolis algorithm, and apply the periodic boundary conditions.

### 3.4 Computation of the system’s properties

In order to have some results, we have to address the computation of some properties of the system, as are the radial distribution function or the energy per particle. We will describe now how we have implemented this calculations in our code.

#### 3.4.1 Radial distribution function

An interesting property of the system to know is the radial distribution function $g_2(x) = \langle \rho(0) \rho(x) \rangle$, since we can infer from it how the particles are distributed all along the boxlength.
In order to compute it, we use the estimator in equation eq.2.23 discussed in past sections. We measure the relative distances between all pairs of beads of different particles (this is, same bead index for different particle index) and build an histogram (see figure 3.10). After doing so during the movement is running, we also have to normalize it.

We could, in principle, compute the radial distribution function by looping over a single bead index of all particles, but we do it over all beads so we obtain better statistics. Hence the normalization of \( g_2(x) \) has also to take into account this extra loop.

\[
\text{RDF } g(r) = \frac{1}{L^2 N \text{ bio}} \sum_{i \neq j} \frac{1}{N \text{ links}} \sum_{i=1}^{N \text{ part}} \frac{1}{N \text{ part}} \text{ abs}(F_{i,j} F_{j,i}) \text{ if } (x_{rel} > 5 \times L) \text{ then } x_{rel} = L - x_{rel} \text{ end if } \]

\[
\text{int} = \text{int}(x_{rel}/dx) + 1 \quad \text{RDF}(\text{int}) = \text{RDF}(\text{int} + 1) \quad \text{count}_{g} = \text{count}_{g} + 1 \quad \end{do}
\end{do}

Figure 3.10: Computation of the radial distribution function

### 3.4.2 Energy per particle

Knowing the energy per particle is important not only for its own intrinsic importance, but also it is useful if we want to know wether we are using a correct number of beads in our simulation or not. For the total energy per particle computation, we make use of the thermodynamic estimator:

\[
\frac{E}{N} = -\frac{1}{NZ} \frac{\partial Z}{\partial \beta} \quad (3.5)
\]

Since the total energy per particle needs such a large amount of time to be computed, and we want to know its average in time, we will adress it only every 1000 movements (this number can be modified directly in the energy routine), so we are sure that the configuration of the system will have fluctuated.

Note that there are three terms in the expression. The first one is \( M \) times the energy of a classical ideal gas, and the following ones

\[
\sum_{j=1}^{M} \frac{(x_{j+1} - x_{j})^2}{4 \lambda \tau^2} \quad (3.6)
\]

the kinetic part (single particle interaction) due to the springs between beads and

\[
\sum_{j=1}^{M} \frac{\partial U(x_{j+1}, x_{j}; \tau)}{\partial \tau} \quad (3.7)
\]

the potential part (two body interaction).

Both the classical gas and single particle terms are easy to compute by just applying the equation eq. 2.27, see figure 3.11.

For the potential energy we have to use the already discussed approximation for the term \( \text{erfc}(u) \exp(u^2) \) eq. 2.33, and run an additional loop for every particle interaction, see figure 3.12.
\[ E_{\text{sp}} = 0.0 \]
\[ x_{r2} = 0.0 \]
\[ \lambda_{mb} = h^4 b/(2TS(N_{\text{links}} + 1, i_n)) \]

\[ \text{do } i_{b} = 1, N_{\text{links}} \]
\[ i_{bpi} = i_{b} + 1 \]
\[ \text{if } (i_{b} \leq N_{\text{links}}) \text{ then} \]
\[ i_{bpi} = 1 \]
\[ \text{endif} \]
\[ x_{rel} = (F_{i_{b}, i_{n}} - F_{i_{bpi}, i_{n}}) \]
\[ \text{if } (\text{abs}(x_{rel}) \gt (L/2)) \text{ then} \]
\[ x_{rel} = 1 - \text{abs}(x_{rel}) \]
\[ \text{endif} \]
\[ x_{r2} = x_{r2} + (x_{rel} \times 2) \]
\[ \text{enddo} \]
\[ x_{r2} = x_{r2}/N_{\text{links}} \]
\[ E_{sp} = x_{r2} / (4 \times \lambda_{mb} \times \tau_{\text{au}} \times \tau_{\text{au}}) \]

Figure 3.11: Computation of single particle energy term

\[ n_{lp} = M_{r} \times (x_{rel} \times y_{rel} + \text{abs}(x_{rel} \times y_{rel})) \times \text{fup}/(\tau_{\text{au}} \times 1.5 \times h^2 \times b) \]
\[ n_{lp} = 1.5 \times \text{fup}/(\tau_{\text{au}}) \]
\[ n_{sp} = \text{sqrt}(M_{r}/3) \times (q \times \tau_{\text{au}} - \text{abs}(x_{rel}) - \text{abs}(y_{rel})) \]
\[ \times (2 \times \text{fup} - 5/\text{spi})/(h^2 \times b) \]
\[ d1p = \exp(M_{r} \times x_{rel} \times y_{rel} + \text{abs}(x_{rel} \times y_{rel}))/((h^2 \times b \times \tau_{\text{au}})) \]
\[ d2p = q \times \text{sqrt}(p \times M_{r} / \tau_{\text{au}}) \times \text{fup}/h^2 \]
\[ n_{lm} = M_{r} \times \text{fup} / (\tau_{\text{au}} \times 1.5 \times h^2 \times b) \]
\[ n_{lm} = 1.5 \times \text{fup}/(\tau_{\text{au}}) \]
\[ n_{lm} = M_{r}/3 \times (q \times \tau_{\text{au}} - \text{abs}(x_{rel}) - \text{abs}(y_{rel})) \]
\[ \times (2 \times \text{fup} - 5/\text{spi})/(h^2 \times b) \]
\[ d1m = \exp(M_{r} \times x_{rel} \times y_{rel} + \text{abs}(x_{rel} \times y_{rel}))/((h^2 \times b \times \tau_{\text{au}})) \]
\[ d2m = q \times \text{sqrt}(p \times M_{r} / \tau_{\text{au}}) \times \text{fup}/h^2 \]
\[ dU = dC + q \times \text{sqrt}(p \times M_{r} / \tau_{\text{au}} / 2) \times (n_{lp} + n_{2p} + n_{3p}) / ((d1p + d2p)) \]
\[ dU = dU \times q \times \text{sqrt}(p \times M_{r} / \tau_{\text{au}} / 2) \times (n_{lm} + n_{2m} + n_{3m}) / ((d1m + d2m)) \]

Figure 3.12: Computation of two-body energy term
Chapter 4

Results

We have applied our code to the study of the total energy per particle and the radial distribution function of the already described system. This chapter is devoted to show the results obtained with our PIMC simulations, contrasting them with both experimental and theoretical results, when possible.

4.1 Observing quantum particles

First of all, we want to illustrate how the path integral formalism can be observed from our results, by means of some world lines. In these world line diagrams, we show how the one dimensional system evolves in time, and how we can distinguish between more classical and more quantum regimes.

In the following figure, we plot the \( x \) position of each bead of a single quantum particle as a function of time.

![Figure 4.1: World line diagram of a single quantum particle](image)

We can observe here how different beads follow different paths in real time, but without separating too much. This is interpreted as the delocalization of the quantum particle. As we have already discussed in past chapters, in the path integral formalism each bead, this is, each path in a different imaginary time, can be interpreted as a possible path that the particle could follow in order to go from position A to B, and these paths that differ the most from the classical one (the one that minimizes the action) are less probable to be followed.

In this plot we have simulated a single particle without any external interaction (and, for sake of simplicity, without thermal fluctuations, this is, without random center of mass movement) so the expected classical movement of the particle would be to stay at the same point, which in the world line diagram would be represented by a straight line. Hence, some beads move away from the center point of the \( x \) axis, but without getting too far away from it.
4.1.1 Effects of mass and temperature

One now may want to address the question of how do the mass of the particle and the temperature of the system affect this world line diagram. Quantum regime is mostly observed in very cold systems of very tiny particles with very low mass: electrons' mechanics, for example, are much worse described by classical approaches than protons', or interesting quantum properties such as superfluidity or superconductivity appear (mostly) at temperatures very close to the absolute zero.

To see the effect of the mass, one could also recall Heisenberg’s uncertainty principle:

\[ \Delta x \Delta p \geq \frac{\hbar}{2} \]  \hspace{1cm} (4.1)

So from equation 4.1, delocalization in space has to decrease with the mass of the particles considered, since momentum is proportional to it. In our path integral formalism, this should be translated in wider polymers of those less massive particles.

We can observe this property in the following world line diagram fig. 4.2, where we plot three different particles with increasing values of mass. Again, for sake of simplicity, we do not consider interactions between them nor thermal fluctuations.

![Figure 4.2: From top to bottom: \( m_1 = 10, m_2 = 1, m_3 = 0.1 \).](image)

As expected, we see how delocalization of particles (or, equivalently, the width of the polymers) is smaller for more massive (more classically approachable) particles.

Also, the same effect takes place when increasing temperature. In the following diagram, we compare two simulations of the same system (again, of three particles with different mass), but at two different temperatures.

![Figure 4.3: Effect of temperature on a quantum system.](image)

And, effectively, decreasing temperatures make the polymers wider (more delocalization, or more quantum-like behaviour).
4.1.2 Reflection and transmission

Two other interesting quantum properties that we can observe via these world-line diagrams are transmission and reflection. For the study of these effects, we consider two particles in free space. Since we are dealing with contact interactions (recall the hamiltonian in equation 2.20), and modeling the two body system from a reference frame where one of the particles is at rest, the resulting system would be equivalent to that of a particle moving freely in space, with a delta potential barrier at some point, being its hamiltonian:

$$H^{rel} = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} + g\delta(x)$$ \hspace{1cm} (4.2)

This kind of typical academic systems has been widely studied and can be easily found in the literature [7]. The point is that, as it is well known, in such a quantum system with a delta barrier the probability of the particle to be transmitted (this is, trespassing this infinite barrier) is not zero, but has, for the hamiltonian in equation 4.2, the analytical expression:

$$T = \frac{1}{1 + \frac{m}{2\hbar^2} \frac{g^2}{E}}$$ \hspace{1cm} (4.3)

Figure 4.4: Transmission T (blue line), and reflection R (red line) coefficients, as a function of the interaction strength g

Being $T$ the probability of the particle to be transmitted and $R = 1 - T$ the probability of being reflected. $E$ is the energy of the particle and $g$ the interaction strength.

Figure 4.5: Comparision of world-line diagrams for low (top plot) and high (bottom plot) interaction strengths
Thus, taking the limit for high and low interaction strengths one finds:

\[
\lim_{g \to \infty} T = 0 \quad \text{(4.4)}
\]

\[
\lim_{g \to 0} T = 1 \quad \text{(4.5)}
\]

So, for very high interaction strengths, particles are fully reflected (no transmission effects take place) [3], so the initial ordering of the particles remains unchanged during time evolution [8]. In the other hand, for lower values of \( g \) transmission is permitted. See figure 4.5 where, in order to be easier to see how particles are reflected and transmitted, we have used in this simulation high temperature, so their delocalization is lower.

### 4.2 Weakly interacting gas

The first case we may address is the weakly interacting gas, this is, almost fully transmitting regime.

#### 4.2.1 Free particles

As a first approach, we want to study the trivial case where we have non-interacting particles, this is \( g = 0 \). For this case, we recover, within a very small statistical error, the theoretical value for the total energy per particle given by statistical mechanics:

\[
\left\langle \frac{E}{N} \right\rangle = \frac{1}{2} k_B T \quad \text{(4.6)}
\]

![Energy per particle in non-interacting regime. The dashed line is the theoretical value, while PIMC results are represented with blue circles](image)

Figure 4.6: Energy per particle in non-interacting regime. The dashed line is the theoretical value, while PIMC results are represented with blue circles

#### 4.2.2 Low interaction in cold systems

In cold systems, the interaction energy per particle reads:

\[
\left\langle \frac{E_{\text{int}}}{N} \right\rangle = g_2(0) \frac{g}{2n} \quad \text{(4.7)}
\]

where \( g_2(0) \) is the radial distribution function evaluated at \( x = 0 \), \( g \) is the interaction strength and \( n \) is the density of particles.
It is also known that, for low interaction strengths, the value of the radial distribution function at \( x = 0 \) can be approximated by:

\[
g_2(0) \approx n^2
\]  

(4.8)

Hence, by combining both equations 4.7 and 4.8, the mean total energy per particle in the low interacting, low temperature regime will be a linear function of the density, starting at the free-particle energy of an ideal gas:

\[
\left\langle \frac{E}{N} \right\rangle = \frac{1}{2} k_B T + \frac{1}{2} g n
\]  

(4.9)

Figure 4.7: Comparative of the total energy at different temperatures and with different \( g \).

In figure 4.7 we can see how, by lowering the value of \( g \), and for different values of the temperature, stright lines as a function of the density and starting from the free-particle energy point are recovered. Effectively, the steepness decreases with the value of \( g \), and would continue to do so until we reached \( g = 0 \), for which we would have a flat line, independent of the density, corresponding to the energy of free particles discussed in the past section.

Figure 4.8: Radial distribution functions for \( g=2, g=1, g=0.1 \), in ascending order
For this regime we also recover the expected radial distribution function \[9\], which we plot in
figure 4.8, for different values of the interaction strength, \(g\). The initial value of these correlation
functions can be obtained within the Helmann-Feynman theorem’s frame.

4.2.3 Ideal gas regime

In a system of low interacting, cold gas, we expect the interacting energy to be of the same order
than the thermal energy, thus both of them contributing to the total energy per particle as seen
in section "Low interaction in cold systems".

\[
\langle E_N \rangle = \frac{1}{2} k_B T + E_{\text{int}} (n, g, T) \quad (4.10)
\]

Nevertheless, if we take a closer look to the figure of this section where we plotted the energy at
low values of both \(T\) and \(g\), fig. 4.7, we can notice that, for higher values of the interaction strength
(more quadratic lines), the curves increase slower with the density of particles when working with
higher temperatures, than at colder regimes. This is, for higher temperatures, the interaction
energy (which is the only part of the total energy that could, at some point, depend on the density,
see equation 4.10) is much less significant than the intrinsic thermal energy: \(k_B T \gg E_{\text{int}}\).

Hence the total energy per particle can be approximated with that expected for an ideal gas:

\[
\langle E_N \rangle \approx \frac{1}{2} k_B T \quad (4.11)
\]

![Figure 4.9: Total energy per particle reaching the expected ideal gas’ energy](image)

Also, it has to be noticed from the discussion above, that, for higher densities, the temperature
that has to be reached in order for the total energy to be well approximated with that of an ideal
gas, increases. This effect can be better observed in figure 4.10, where we have plotted the relative
error between the ideal gas’ theoretically expected energy and the energy of a system with a low
interaction strength and for different values of the density, obtained with our PIMC code.

In figures 4.9 and 4.10, blue circles, red triangles and yellow squares correspond, respectively,
to the simulations carried out considering systems consisting of \(N = 4\), \(N = 6\) and \(N = 8\) particles.
As we could expect, correlations and, hence, interaction energies, are higher for increasing densities,
so also does the needed temperature for entering the ideal gas regime.
4.3 Highly interacting gas

Now we may address the study of high interparticle interaction strength, this is, fully reflecting regime (see eq. 4.4). In this approach, we can also do some extra approximation in the computation of the action, especially in the two-body thermal density matrix term eq. 3.2.

Being \[ u = \sqrt{\frac{\mu^2}{2\tau} + \frac{|x^{(i)}| + |x^{(i')}| + g\tau}{\hbar}} \], for large \( g \) one finds:

\[ u \approx \sqrt{\frac{\mu\tau g}{2\hbar}} \]  

(4.12)

And, using the known limit \( \lim_{u \to 0} [\text{erfc} (u) \exp (u^2) u] = \frac{1}{\sqrt{\pi}} \), along with equation 4.12, the expression of the thermal density matrix 3.2 can be reduced to [3]:

\[
\bar{\rho}^{rel}(x_j^{(i)}, x_j^{(i')}; \tau) = \begin{cases} 
1 - \exp \left( \frac{\mu(x_j^{(i)} - x_j^{(i')})^2}{\tau\hbar^2} \right) & \text{for } x_j^{(i)} x_j^{(i')} > 0 \\
0 & \text{for } x_j^{(i)} x_j^{(i')} \leq 0
\end{cases}
\]

(4.13)

4.3.1 Ideal gas with high interactions

The first question we may have with respect to the highly interacting gas is whether there exists or not, as we found with smaller values of the interaction strength \( g \), an ideal gas regime. To do so, again we fix a high value of \( g \) and, for different values of the density of particles, we run some simulations for increasing temperatures.

Effectively, we found that for high temperatures, the bose gas’ energy can be approximated by that of an ideal gas.

Nevertheless, we should note that, since now the interacting energy is much stronger, we can assume the limit in eq. 4.11 only for temperatures much higher than the ones needed in the weakly interacting case.
4.3.2 Strong interactions at lower temperatures

Until now, we have seen how our code works properly and is able to recover, within an acceptably small error, the expected values for a full range of temperatures when dealing with weak interactions, and also at high temperatures with strong ones.

Possibly, the strong interacting, cold regime is the most interesting one since quantum properties start to appear and to take an important role in physical systems. Nevertheless, our PIMC code does not work right in this more interesting conditions, possibly due to a fail in the sampling of the two-body density matrix term, that makes the code fail and give wrong results when the interaction between particles is strong enough (revisions of the code and method in order to try to fix it are currently taking place).

For instance, we can see that the code starts to fail for high values of $g$ by comparing the radial distribution function, $g_2(x)$, which in such highly interacting systems can be theoretically computed as [9] [11]:

$$g_2(x) = 1 - \left( \frac{\sin(\pi nx)}{\pi nx} \right)^2$$  (4.14)

Figure 4.12: Comparison of the theoretical and the obtained with our PIMC code radial distribution functions. Solid line is theory and triangles PIMC results
So, by plotting both $g_2(x)$, the one given by our PIMC code and the theoretically expected, we find the comparison in figure 4.12. The shape in both curves is similar, but PIMC’s one tends to go higher at intermediate distances, and then does not reach the asymptotically value of one, but goes below it.

This fact is also noticeable in the radial distribution functions presented in the section *Low interaction in cold systems* figure 4.8. When one looks their shapes with more attention, is able to see that they are not totally correct: for instance, they go above one at some points at half the total considered distance, when they are supposed to reach this value only asymptotically.

**A qualitative approach to Reflection-Transmission transition**

Nevertheless, our PIMC code does give us some results that make it possible, at least in a qualitative way, to take a closer look at some properties. For instance, when applying it to the study, as a function of the interaction strength $g$, of the total energy per particle of systems with different densities and at different temperatures, the following results are found (see figure 4.13).

![Figure 4.13: Energy per particle as a function of the interaction strength $g$](image)

Where, from top to bottom, the curves represent the total energy per particle, as a function of $g$, obtained from the simulation of the following systems: $T = 5$ and $N = 4$ (red curve), $T = 1$ and $N = 4$ (blue curve), $T = 5$ and $N = 3$ (purple curve), $T = 1$ and $N = 3$ (yellow curve).

From these curves, we can remark some important aspects:

1. All curves start, for $g = 0$, at the energy expected for an ideal gas, as seen in section *Weakly interacting gas: Free particles*.

2. Energy first increases linearly with $g$, and then collapses into a given value, reaching a steady state.

3. The steady, collapsed value of the energy is higher for higher densities at same temperature.

4. The steady, collapsed value of the energy is reached at higher values of $g$ for hotter systems with the same density of particles.

And, from this facts, we can extrapolate a transition from an *increasing energy* state to a *collapsed* one. This transition takes place, as we conclude from the discussed plot, at higher values...
of $g$ in hotter systems, and the final energy is higher for more dense systems at same temperature. In fact, this transition between these two very differentiate states has the same properties of that given when going from the transmitting to the totally reflecting regimes, explained in section *Observing quantum particles: Reflection and transmission*. When particles are in the transmitting regime (this is, low $g$, see equation 4.5) energy just keeps increasing with the interaction strength, since they can move freely (freelier for lower densities, since they are more separated). Then, once they enter the fully reflecting regime, the energy cannot increase more with higher values of $g$, since they are completely confined [3], and the only way to make this energy higher is by increasing its thermal energy, so this collapsed energy will be higher for hotter temperatures. Recall that, since we are working with zero range interactions, the interacting energy is only proportional to the number of collisions between particles per unit time (and also, of course, to the absolute value of $g$).

Actually, this energy shape as a function of $g$ is, more or less, the theoretically expected for this kind of systems. Nevertheless, the total energy should reach, at this collapsed point, the Fermi’s energy for the given parameters [9] [11].

$$\langle \frac{E}{N} \rangle = E_F = \frac{\pi^2 \hbar^2 n^2}{6m} \quad (4.15)$$
Chapter 5

Conclusions

We have developed a code that simulates mixtures of one dimensional Bose gasses at finite temperatures and with contact interactions within the PIMC formalism. Although our code presents failure when dealing with strong interactions at low temperatures (this fact is currently being fixed), it also gives us correct results for more conservative systems.

From the results obtained we are able to clearly identify some different scenarios as are the ideal gas regimes for weak and strong interacting particles. From the results of the regime where the code does not work properly, we can, nevertheless, at least in a qualitative way, identify a transition between fully reflecting and transmitting states. We also are able to show how some basic properties of quantum particles behave as a function of mass and temperature, by means of the characteristic classical isomorphism of the path integral monte carlo method of polymers.

It is also noticeable the numerical problem solved for the computation of the energy and the two-body density matrix, for which we had avoided the explicit evaluation of the complementary error function and the exponential of a quadratic, positive term, since no previous references on how to deal with it where found.

Finally, aside of the already discussed needs of the code to be fixed, we have also proposed some ways to improve it, from more complex and accurate approximations of the thermal density matrix, to other properties that could be computed in order to the study to be more extensive.
Bibliography

[14] N. Metropolis et al., Journal of Chemical Physics, 21, 1087 (1953)