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MONTE CARLO SIMULATION OF RECENT
EXPERIMENTS WITH ULTRACOLD DIPOLAR
ATOMS IN ONE DIMENSION

TFG

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1 Introduction

The objective of this document is to define in an accurate and detailed way all the factors related with the management of this final degree project (TFG from now on), of the A modality. These factors will be: the context and the motivation of the problem to solve, the time and the costs associated to its development. A temporal planning is formulated and the costs are explained in a budget with a control plan.

1.1 Context

The comprehension of the world of quantum physics is one of the great achievements in human history, as it provides the microscopic basis for understanding natural phenomena. Indeed, as mentioned in Ref. [3], quantum physics can be successfully used to explain properties of the atom, the chemical bond, molecules, the interaction of light with particles, matter, and a large number of different things. Although quantum physics describes the world on atomic scale, we can observe its consequences on a macroscopic scale in thermal properties (such as radiation), optical (such as colors), electrical (such as between insulators, metals, and semiconductors in crystalline solids, the solids which have a structure periodic and sorted), and magnetic (such as ferromagnetism, antiferromagnetism, and other magnetic orders of matter). Quantum physics in turn has important technological applications such as the invention of the transistor and therefore the computer and is the basis of most of the high electronic technology that we use today.

A fundamental idea is the wave-matter duality consisting in that quantum particles also behave as waves. This idea was formulated by De Broglie who propose that the momentum of a particle, which is classical description is the product of mass and velocity ($p = m * v$), is inversely proportional to the wavelength ($p = h/\lambda$). The proportionality factor h is the Planck constant. This hypothesis has been confirmed numerous times in interference phenomena.

In this context Newton equations of motion might become insufficient when applied to description of the evolution of quantum particles. Instead, the propagation of the wave function associated with a particle should be described by the Schrödinger equation.

Unusual consequences such as Heisenberg's uncertainty principle, the tunneling effect, the quantization of properties such as energy or momentum and in many-particle systems their classification into *bosons* and *fermions* are deduced from the theory of quantum physics. Which are the basis for understanding the world around us.

1.2 Useful definitions

Here will be some useful definitions, in order to make the description of the problem more understandable, as there will appear some things related to quantum

physics, and there are some terms which are not easy to understand if they are not explained.

1. **Standard model of elementary particles**[15]: This are subatomic particles which are not composed of any other particle. Particles currently thought to be elementary include fermions which are the ones that form the matter, and bosons which are the ones that generate the force between interactions. See Figure 2 for more details.
2. **Wave functions:** Quantum mechanics cannot predict the exact location of a particle in space, only the probability of finding it at different locations, we can see an example of wave function on Figure 1.
3. **Fundamental interactions:** There are four fundamental interactions known to exist: the gravitational and electromagnetic interactions, which produce significant long-range forces whose effects can be seen directly in everyday life, and the strong and weak interactions, which produce forces at minuscule, subatomic distances and govern nuclear interactions, this interactions can be attractive or repulsive, except the gravitational one which is not clear if there exists one repulsive, as it is one of the mysteries that scientists have nowadays.

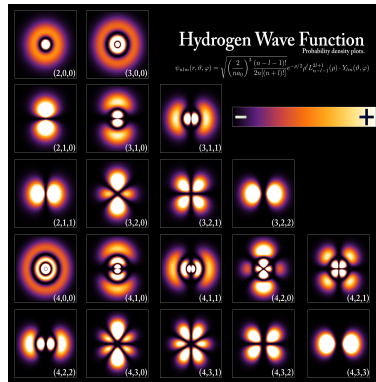


Figure 1: Wave function of an electron in an hydrogen atom

1.3 Formulation of the problem

Nowadays, there are numerous experiments with quantum matter. Quantum many-body scars, long-lived excited states of correlated quantum chaotic systems that evade thermalization (a body that reaches thermal equilibrium through mutual interaction), are of great fundamental and technological interest.

In this project I am going to carry out a Monte Carlo simulation of one recent experiment with ultracold atoms. If the temperature is very low the motion of

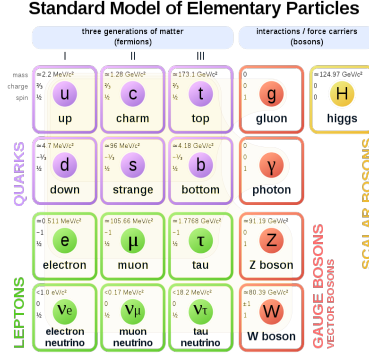


Figure 2: Standard Model of Elementary Particles

atoms should be described as motion of waves and described by the wave function ψ . The probability of finding a particle in a certain place is then described by the square of the wave function, $|\psi|^2$. There are two possible symmetries in exchange of identical particles, when positions of any two particles are interchanged the wave function (i) does not change sign, $\psi_B(x_2, x_1) = \psi_B(x_1, x_2)$ (ii) changes its sign $\psi_F(x_2, x_1) = -\psi_F(x_1, x_2)$. In both cases the square of the wave function $|\psi(x_1, x_2)|^2$ does not change. In the first case the particles follow Bose-Einstein statistics and the second one the Fermi-Dirac statistics. The first type of particles (bosons) are allowed to occupy exactly the same wave as the temperature is lowered. In particular, at temperatures as low as $10^{-9}K$ above the absolute zero, the bosons form a Bose-condensate, i.e. all particles are participating in the same macroscopic wave and their properties are described by exactly the same wave function. This function is known as a condensate wave function.

In recent experiments, temperatures as low as $10^{-9}K$ have been reached allowing an experimental investigation of the properties of quantum particles. Also the particles can be confined to a waveguide geometry, where the motion is allowed only along one direction[8]. In practice, the external potential is applied and the atoms are shaped into an array of tight tubes, as the ones on Figure 3.

A peculiarity of a one-dimensional world is that the Bose-Einstein condensation is absent even at the absolute zero. As a result, alternative methods are needed to describe the system properties. A possible choice are quantum Monte-Carlo methods.

In experiment [9], ultracold dipolar atoms are studied in one-dimensional geometry. A magnetic field is applied to control the interactions between the atoms, by tuning the strength of the short-range interaction by using the Feshbach resonance technique. In practice this means that the strength of the short-range interaction can be arbitrarily tuned to any value ranging from minus to plus infinity. In addition there is a dipolar interaction and its strength can be modified by changing the angle θ between the orientation of dipoles and

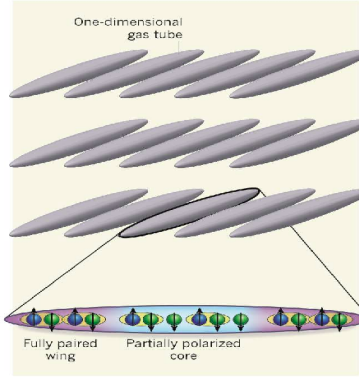
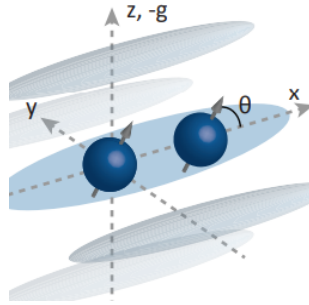


Figure 3: 1D gas tubes

the direction of the tube as we can see in Figure 4.

Figure 4: Dipoles interacting inside the tube forming an angle θ with the tube

A peculiarity of the one-dimensional geometry is that a gas with infinitely-repulsive short-range potential is stable. In this case the Bose atoms acquire fermionic properties. Indeed, two fermions cannot stay in exactly the same place due to the Pauli exclusion principle, $\psi_F(x_1 = x_2) = 0$. Instead two bosons with an infinite repulsion neither can stay in the same place, $\psi_B(x_1 = x_2) = 0$, due to the interaction potential. As was shown by M. Girardeau[7] in a one-dimensional system of N atoms, the bosonic wave function $\psi_B(x_1, \dots, x_N)$ and the fermionic one $\psi_F(x_1, \dots, x_N)$ are related as $\psi_B(x_1, \dots, x_N) = |\psi_F(x_1, \dots, x_N)|$. Such a system is known as a Tonks-Girardeau gas and recently has been experimentally realized[11].

In the recent experiment, the one-dimensional dipolar gas was set in motion in a weak harmonic trap. The gas gently “breathes” by periodically changing its size. The frequency of the breathing mode has been measured. For a moment, there is no theory describing well the obtained experimental results. The scope of the TFG is to provide an ab-initio modelling of the one-dimensional dipolar gas under realistic conditions. In particular, the ground-state energy and the

pair-distribution functions will be obtained numerically as a function of the density. The obtained energy dependence on the density (equation of state) will be used in order to calculate the breathing frequency in a trap.

The properties of the quantum system are governed by the many-body wave function, which we chose in pair-product (Bijl-Jastrow) form, $\psi(x_1, \dots, x_N) = \prod_{i<j}^N f(x_i - x_j)$. In particular, for Tonks-Girardeau regime, the Jastrow term is known exactly, $f_2(x) = \sin(\pi x/L)$ [7]. In other cases, the Jastrow term will be found as a solution to the two-body Schrödinger equation with the realistic interaction potential taken from Ref. [9].

1.4 Actors implicated

In this project there are few actors implicated:

1. *The staff of the project.* We are going to develop the project and we have to finalize in time this project and obtain a result of quality.
2. *The authors of the experiment.* They made a practical experiment and the results that we can obtain can be useful for them.

2 Justification

The quantum world has become one of the fields of the most interest that humanity has nowadays, so as this project treated a part of that world it was a very interesting topic, it merges computer science and physics, two of the things I enjoy the most.

As the Monte Carlo algorithm can be implemented in the majority of programming languages, I decided to use Python, as it is one comfortable language to program with and it has a huge quantity of libraries that may be useful for developing some part of the code.

3 Scope

3.1 Objective

The goal of this TFG is to be able to realize a simulation of the experiment [9]. For a moment there is no theory which is able to quantitatively describe the experimental results for the breathing mode. The goal is to perform an *ab initio* modeling based directly on the microscopic model. Quantum Monte Carlo code will be written to calculate the energy and correlation function of the system.

3.2 Sub objectives

The sub objectives that must be achieved during the project are this:

1. Develop the model for the simulation
2. Develop Quantum Monte Carlo code for being able to obtain results
3. Obtain the energy of the system as function of linear density
4. Obtain correlation functions, such as the density-density distribution function $g_2(x)$
5. Obtain the frequency of the breaching oscillations from the energy of the system

3.3 Requirements

This project requires a quick development of the code in order to be able to obtain the numerical values that must be obtained, as once the code will be developed there will be some time that will be spend on finding the results and interpreting them. Also, some knowledge of the quantum field must be understood in order to manage with the results once they have been obtained.

3.4 Obstacles

I identified two obstacles that make more difficult the completeness of the goals:

1. *Inexperience.* The author of this work have never worked on the quantum world, so this can be a difficult topic to manage with.
2. *Documentation.* The actual regulation of the TFG requires a lot of documentation, which is a hard part of the project, and the explanations must be very clear.

3.5 Risks

These are the risks I consider they might appear during the project:

1. *Time management.* On the period that the author is doing this TFG, he is doing an English course and three subjects more at the same time. For this reason, lots of time difficulties can appear during the project.
2. *Accidents.* Even though it is not usual to have an accident, it could happen and this would be an important setback to the project, due to the brief time that we dispose with.

4 Methodology and monitoring

4.1 Work methodology

This is a complex project for different reasons:

- It combines different type of thematic such as randomized algorithms, from the Computer Science branch, and quantum physics concepts and formulas which are not explained in this career.
- The software that will be created must be of low consumption and it must be able to give a response in a reasonable time.
- The results obtained are a big quantity of results, so it should be a big dedication to understand the results and corroborate them.
- Only a person is working on this project (with the manager's support), which theoretically has to dedicate 450 hours during three months.

This is the first TFG of this author, who has never worked on quantum physics nor has done any kind of simulation. However, he has done some subjects on which some topics of this work appeared. So, it will be necessary to have a work methodology which does not require a previous knowledge of the things that will be done and that allows to define, in a dynamic way the tasks to realize.

4.2 Monitoring

In order to verify that the development is adapting to the requirements of the project and to be able to correct without delay the deviations that could appear, we will follow the monitoring of the project with weekly meetings, in which, we will analyze the progress of the memory, the difficulties that have appeared, the improvements that can be applied and the achievements of the objectives and sub-objectives that we have fixed, with the help of the indicators.

5 Temporal extension

I have predicted that this project will require 450 hours of dedication (25 hours/ECTS by 18 ECTS) during 12 weeks. Even though the basic data of the TFG was accorded when the inscription of the TFG, the execution of it didn't start until the 17th of February of 2021, when the informative session of GEP. My prevision is to have finished the project by the end of May of 2021.

The reason for anticipating the end of the work by those days is that the follow-up meeting is the 28th of March, so the project should be finished or nearly finished, if some risk of the project has become a problem, to give a final review, and then deliver it on time. As the lecture of TFG of June of 2021 starts on the 28th of June of 2021, so the work should be done, and the memory ready for no more after the 21th of June of 2021, as it has to be delivered at least one week before the lecture.

6 Staff and materials

As for the staff, this project requires one manager of the work, one programmer and one analyst, but in this case the role of the analyst will be distributed onto

the programmer and the manager, so 2 people will be enough to work on this project, because of the tasks that have to be developed. Specifically:

- The project manager who is in charge of the setting of the scope and the project characteristics, to control how they are realized, to coordinate the members of the work team and to meet with the vendor in order to have him on day with the project evolution.
- The programmer who has the role of programming the code for the simulation, and to ensure the correct operation of the code.
- The analyst who will determine the results of the code of the programmer and suggest if something is not going as it should be, and to reason the correct results obtained with the code.

The materials that the project will need are:

- Two personal computers (for the workforce).
- One work space with the Internet. Some documentation about the experiment to understand it well.

7 Phases of the project

This project have two main parts: the development of the quantum Monte Carlo code (MC) and the documentation elaboration (D). In the work, both parts will be done in a more or less parallel way, once the project has been planned. What is more, there will be weekly meetings of monitoring (M) during the project.

On the hand of the development of the code we can identify four phases:

- Previous study (ME)
- Model simulation (MD)
- Implementation (MI)

The realization of the documentation consists of one part, because everything has time during all the length of the project and only consists of two tasks.

The monitoring meetings will not be divided by phases, because the meetings are quite homogeneous: on each meeting it will be analyzed what has been done during the last week, and will be planned what has to be done for the next one.

8 Tasks descriptions

8.1 Previous study (ME)

- **ME1: Scope and requirements.** As this is a complex project it is essential to build stronger foundations for the work and establish clearly what we want to build and what specific characteristics it must have to suit our needs.

- **ME2: Temporal planning.** Once we have decided what to do, we will have to decide how we will distribute the project in tasks and what dedication in time we will allocate to each one.
- **ME3: Budget and sustainability analysis.** With the time planning done, we will decide which profiles of people would be in charge of carrying out the project if it is a project carried out by staff of a company or public administration and what the cost would be. We will also analyze the sustainability effects of the project.
- **ME4: Measurement of electric consumption.** When running the simulation some energy will be spent on that process, if it takes lots of hours to finish the execution, it can become a considerable spent of energy, but nothing compared to a server for example.

8.2 Model simulation (MD)

- **MD1: Model design.** We have to establish the model: how many atoms are there, where are they allocated, how big is the box where the simulation will take place, and some other parameters that can be tuned.
- **MD2: Algorithms design.** We have to establish how the interactions will take place, and what will be the resulting model after it, also Monte Carlo method must be programmed to obtain the results.

8.3 Implementation (MI)

- **MI1: Implementation of the code that generates the model.** We will develop the code which will generate the model, so then it will be used for the simulation.
- **MI2: Implementation of the Monte Carlo code.** We will use the model to run the simulation using the Monte Carlo method, it will generate the results that we wanted to obtain.

8.4 Tests (MT)

- **MT1: Partial tests in the development environment.** As we develop the software, I will be testing to verify that the code is working properly and to be able to correct some possible errors.
- **MT2: Final tests in the development environment.** Once the software is full developed, it will be tested with everything, as it was the final result, to find some final errors and have a perfect version of the code.

8.5 Documentation (D)

- **D1: Files of GEP.** I will make files to explain what I have concluded about GEP in relation to the work and then I will merge it, adding in the observations that have been done, in order to have a good base for the memory.
- **D2: Memory.** Although this task takes a very long time, I believe that it doesn't make sense to divide it further: apart from project management information, it's likely that the text is modified or reorganized as the development of the project.

8.6 Monitoring meetings (R)

- **R1: Initial meeting.** At this meeting, I will agree with the project manager on the objectives and project requirements and we will validate that the obstacles and risks of the project are not, in reality, impediments.
- **R2: Ordinary monitoring meetings.** I will meet weekly with the manager in order to review the progress of the project during the previous week, plan what will be done the following week and establish the necessary measures in order to resolve the deviations that are detected.
- **R3: Intermediate tape meeting.** The regulation of TFGs in our faculty requires that the principal and the student meet to evaluate the achievement of the project objectives when approximately half of the work is thought to have been completed.
- **R4: Final meeting.** A pair of weeks before the date of delivery of the memory, I will meet with the manager with three objectives: to validate that the objectives and the requirements have been completed, to solve possible mistakes, or some bad things of the memory and to prepare the oral presentation of the project in front of the court.

9 Dependencies between tasks

The dependencies between tasks of this project are the ones that appear on figure 5 , in which the dependencies end-to-beginning are shown with continuous lines and the dependencies beginning-to-beginning are shown as discontinuous lines.

10 Time dedication to each task

I have made the forecast of the time to dedicate to the tasks thinking in working weeks of 37,5 hours (450 hours between 12 weeks) and basing on the next premises and estimates:

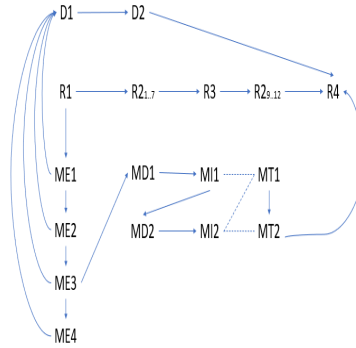


Figure 5: Dependencies between the tasks of this project

- The first three weeks I have to consider the work as a project and write the conclusions obtained from them as main tasks; these occupy a significant part of the time of these weeks and correspond to the project manager.
- The measure of electricity consumption consists of programming a device to give the data or obtain them from a program and store them for study. The code corresponds to the programmer, who can complete it in a day and a half of work; the measure itself lasts a week.
- The analyst and the programmer can design and implement, respectively, each part of the code, in about sixty hours and in about thirty-five hours, given its complexity.
- With regard to testing, we have considered that separate component testing will last, all together, a hundred sixty hours. As it is a very long task, in which the correctness of the code must be proved by understanding of the results and the relation with theoretical physics.
- I have valued that, since memory is the most important testimony of the work that will take place and therefore requires special care, the analyst will spend about ten hours weekly throughout the project.
- Regarding meetings, we consider that an initial meeting, a weekly meeting, and a final meeting, all two hours long, are sufficient to monitor the good progress of the project. The project manager is responsible for the relationship with the client and, for so much so, he must be the one to attend the meetings with him.

11 Task summary table

We show the summary table of tasks to be performed in Table 6. As will be seen in section 14.2, the names of professional profiles come from the sectoral

agreement applicable until 2018 (Resolution of March 18, 2009, of the General Directorate of Labor, which registers and publishes the XVI State collective agreement for consulting and market research and public opinion companies 2009, March 18).

Id.	Task	Hours	Profile
ME1	Contextualization and scope	10	Project manager
ME2	Temporal planning	10	Project manager
ME3	Budget and sustainability analysis	10	Project manager
ME4	Measurement of electric consumption	10	Programmer
MD1	Model design	10	Analyst
MD2	Algorithms design	10	Analyst
M11	Implementation of the code that generates the model	20	Programmer
M12	Implementation of the Monte Carlo code	20	Programmer
MT1	Partial tests in the development environment	90	Analyst
MT2	Final tests in the development environment	60	Analyst
D1	Files of GEP	30	Analyst
D2	Memory	80	Analyst
R1	Initial meeting	2	Project manager
R2	Ordinary monitoring meetings	20	Project manager
R3	Intermediate tape meeting	2	Project manager
R4	Final meeting	2	Project manager

Figure 6: Task summary table

12 Gantt Diagram

The tasks on the Gantt diagram on Figure 7 are represented on a schedule according to the days of the month when they will take place.

Neither the main objective nor the sub-objectives nor the indicators appear in this diagram, for two main reasons.

First of all, the main objective and sub-objectives are very broad. Some of them are character should be taken into account throughout development (security is an example). With regard to the other sub-objectives, we plan to work towards achieving them throughout the four development tasks and we hope that they will be completed by the end of this stage.

Secondly, the indicators are so numerous that it is very difficult for us to determine in what order we will satisfy them and how long it will take us to do so. This also applies, to a lesser extent, to sub-objectives.

13 Risk management

As previously explained in section 3.5, two types of risks are anticipated in our project: the peaks of work of the other activities developed by the author and

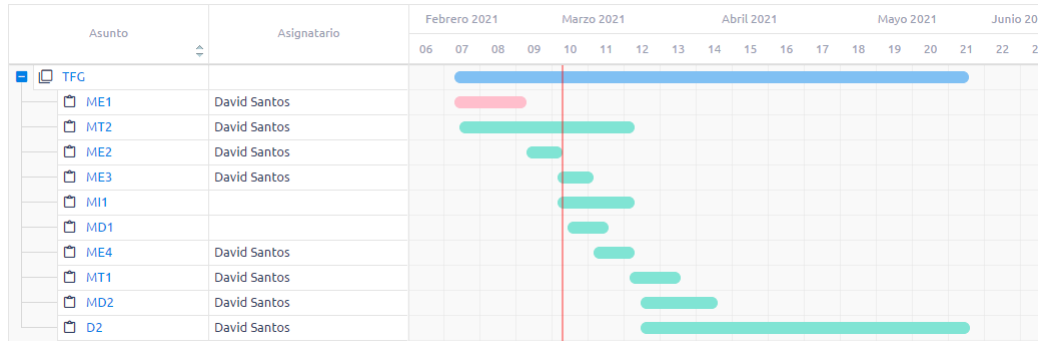


Figure 7: Gantt diagram of the time planning

possible accidents that might happen during the project.

The strategies thought for mitigating the effects of these potential risks are: first, doing an additional dedication to the weeks of low workload, in order to compensate any other week that less hours could be dedicated. Secondly, all the progress done will be automatically saved, so no blackout or strange phenomena that could happen would destroy the job done during hours of work.

14 Budget

14.1 Cost identification

We can consider that all the costs of this project can be classified into the following categories:

- **Staff:** project manager, analyst and programmer.
- **Development:** work space and personal computers for the workforce.
- **Energy:** Electric consumption of personal computers.

14.2 Staff cost

As previously indicated, the project requires one project manager, one programmer and one analyst. The “State collective bargaining agreement for companies consulting and market research and public opinion ” is applicable to the computer science sector.

Since the XVIIth convention does not name the professional categories (Resolution of 22 February 2018, of the General Directorate of Employment, by which the XVII Collective Agreement is registered and published state consulting and market research and public opinion firms 2018, February 22, art. 15), we have used the names of categories of the XVI’e (Resolution of March 18, 2009, of the General Directorate of Labor, which registers and publishes the

XVI State Collective Agreement of consulting and market research companies and public opinion 2009, March 18, art. 15) to identify analyst and programmer jobs. However, when calculating the salaries we have applied the general criteria of the XVII agreement (Resolution of February 22, 2018, of the General Directorate of Employment, by which the XVII Collective Agreement is registered and published state consulting and market research and public opinion firms 2018, February 22, art. 15) instead of the table of equivalences (Resolution of 22 February 2018, of the Directorate General of Employment, by which the XVII state collective agreement of companies is registered and published Consulting and Market Research and Public Opinion 2018, February 22, DT 2) why it provides that equivalences are “only for the purposes of transposition”. We also had in note that the maximum annual working day is 1800 hours (Resolution of 22 February 2018, of the General Directorate of Employment, which registers and publishes the XVII State Collective Agreement of consulting and market research companies and public opinion 2018, February 22, art. 20.1).

Profile	Group	Level	Salary	Quote	Cost/year	Cost/h	Hours	Cost	
Project manager A			-	48.923	14.6769	63.5999	19.33	59	1140.47
Analyst	B	1	28.173	8.4519	36.6249	18.75	320	6000	
Programmer	C	1	27.603	8.2809	35.8839	17.78	71	1262.38	
Total							450	8402.85	

Figure 8: Expected salary costs of the project

As salaries are between the minimum and maximum contribution bases of group 2 (that of engineers (Social Security: Bases and types of contributions 2019 n.d.), workers contribute for their salary. We have applied the limits and types of contributions for 2019 (this year’s ones have not yet been published), which add up to 29.90% [2]. In order not to complicate the calculation excessively, we have assumed who are full - time workers with an indefinite contract (we understand that they are engaged the rest of their working time on other projects). From all that we have exposed, we have calculated the wage costs of the people we work in the project are those in Table 8, which are shown at the activity level in Table 9.

14.3 Development cost

The spaces in which the module would be developed, in a company or public administration must be able to keep all three people on the team throughout the project. On the Internet we found a room of 100 m² for 500 euros / month, with a capacity of about 15 people (Rental of Office in calle Doctor Ferran, 11 b n.d.); a laptop table of 59 euros (FJALLBO Table for laptop - Black - IKEA n.d.); a work chair of the same price (FLINTAN Work chair - Black - IKEA n.d.); a portable holder of 249 euros (Lenovo Ideapad S145-15AST AMD A6-9225 / 8GB / 256 GB SSD / 15.6 PcComponentes.com n.d.) and a rate

Task	Concept	Hours	Cost/h	Cost
ME1	Salary (project manager)	11	19.33	212.63
ME2	Salary (project manager)	11	19.33	212.63
ME3	Salary (project manager)	11	19.33	212.63
ME4	Salary (programmer)	11	17.78	195.58
MD1	Salary (analyst)	20	18.75	375
MD2	Salary (analyst)	15	18.75	281.25
MI1	Salary (programmer)	30	17.78	533.4
MI2	Salary (programmer)	30	17.78	533.4
MT1	Salary (analyst)	100	18.75	1875
MT2	Salary (analyst)	60	18.75	1125
D1	Salary (analyst)	35	18.75	656.25
D2	Salary (analyst)	90	18.75	1687.5
R1	Salary (project manager)	2	19.33	38.66
R2	Salary (project manager)	20	19.33	386.6
R3	Salary (project manager)	2	19.33	38.66
R4	Salary (project manager)	2	19.33	38.66
Total				8402.9

Figure 9: Expected salary costs of the project, separated by activities

1000/500 Mbps Internet connection of 99 euros / month (The best dedicated fiber, with the best guarantee of performance - Fibracat n.d.). The chairs have a 10-year warranty, while the tables and the laptops only have a standard 2-year warranty (Warranty - Support Center - PcComponentes.com n.d. ; Guarantees IKEA - IKEA n.d.): we will assume that this is your life Useful. We consider that in this office people could work in three shifts. In terms of software, this project uses Jupiter, Ubuntu, vim, LATEX, bash and others free, open source software tools, which therefore do not involve any disbursement economics. The costs corresponding to these estimates are those in Table 10.

14.4 Energy cost

Having view the information of the power of laptops (Lenovo IdeaPad S145 - Laptop with technology 39.62 cm (15.6 ") AMD for everyday use - Lenovo Spain n.d.) and Monday's PVPC March 9, 2020 at midnight (PVPC - ESIOS electricity · data · transparency n.d.), we can estimate that the energy costs will be similar to those in Table 6.

Item	Price/u	Capacity/u	Needed capacity	Amortized units	Cost
Office	500	45 (15P, 3T, 1M)	9 (3P, 1T, 3M)	0.2	100
Table	59	72 (1P, 3T, 24M)	9 (3P, 1T, 3M)	0.125	7.38
Chair	59	360 (1P, 3T, 120M)	9 (3P, 1T, 3M)	0.025	1.48
Laptop	249	72 (1P, 3T, 24M)	9 (3P, 1T, 3M)	0.125	31.13
Internet	99	45 (15P, 3T, 1M)	9 (3P, 1T, 3M)	0.2	19.8
Total					159.79

Figure 10: Expected development costs of the project. In this table, “P”, “T” and “M” represent, respectively, people per shift, shifts per day and months

Item	Time	Power	Consumption	Cost/kWh	Cost/h	Cost
Laptop	450h	7.78 W	3500 Wh	0.08798	<0.01	0.31

Figure 11: Energy costs planned for the project

14.5 Contingency

I have included a generous contingency item (30%) in the budget because I do not have it valued lower expenses but also necessary for space and time reasons.

14.6 Unforseens

At section 3.5 I had mentioned different possible risks that might appear on the project: the work peaks of the other activities carried out by the author and possible accidents that might occur.

In the section 13 have been indicated some possible strategies in order to mitigate the effects of the risk: additional working time and auto-saves of the project. As these strategies don't affect the budget they won't be taken into account.

The thing which is included on the budget an item to combat the possible mismatch of results, which is associated with a probability of 10%.

15 Management control

In relation to management control, we thought it is best to take advantage of the weekly meetings to perform it, for two main reasons. The first is that we haven't seen any useful ways to articulate a parallel mechanism to perform this function, but the disadvantage is adding customer interactions even though we already have a weekly meeting there. The second is that in this way we can proactively and effectively correct the deviations we detect in the project while there is time to do so. The way in which we carry out this function will not be elaborated, because we do not need: we will estimate the level of completion of each task and the hours invested in it, we will relate them with the hours we

have planned for the task and we will readjust the planning in case we detect any deviation. In case we detect favorable deviations in the course of the project, we will take advantage of them to advance work; given the risks to the project, we find it risky to expand the scope of the project in the “good” weeks and, for this reason, we will leave the possible extensions for the end (or for a future project).

16 Sustainability

16.1 Thought

I have been aware for years that computer science can have negative and positive implications for people’s lives, in the environment and in the world in general. That’s why I try to take ethics into account and not waste resources both in my private life and in the developments that I do, but I find that society does not give the social and environmental sustainability of projects the importance it deserves. On the contrary, I find that companies place too much weight on economic benefit, but I recognize that I do not master economic analysis.

16.2 Economic dimension

In relation with the economic dimension of the project, these are the conclusions that can be obtained:

- The different development costs have been accounted for: computers for work, office furniture, software, energy and labor.
- The project cost are so reduced. I don’t think there is any way to cut down the cost of the project, and if it was possible it could be counterproductive.
- This project is one simulation of one physics experiment. However, is a project of the UPC.

16.3 Social dimension

The analysis done of the social dimension of this project is the following:

- The project will be developed at the UPC. Currently, in our nearest geographical environment there is a more or less stable socio-political situation. Although there are inequalities and political tensions, this project does not contribute to increasing them. On the contrary, it will help you to improve a tool that can be used by people who cannot finance university studies with the goal of learning to program or improve their skills.
- In the IT sector, as in others considered “qualified”, there is a lot of precariousness, mainly in consulting companies, called “meat”. This is one research of a physics experiment, and no company will take part in

the development of it, so I don't think that this project alters the sector situation.

- In the physics sector, lots of different research is being run all over the world. Technically, this project is not essential, but it will be useful to describe the theoretical part of the experimental results obtained, as well as it would contribute to determining whether the corresponding physical model is fine or it needs some changes.
- Nobody should be harmed for this project, unless someone would like to work on the same project and wanted to be the first to work on it.

16.4 Environmental dimension

In relation with the environmental dimension of the project, the following can be concluded:

- The resources needed for the project are the ones previously indicated. No natural resources are extracted nor substances emitted.
- The activity that will be done is the development of a code, and the understanding of the results, which could be a bit intensive, but it will have a reduced impact to the environment.

17 Monte Carlo method

Once the model is defined we will calculate the system properties (energy, pair distribution function $g_2(x)$, etc) via the Metropolis algorithm [14]. The algorithm consists in generating a sequence of M points (R) in the phase space distributed according to the probability distribution $p(R)$. Here $R = \{x_1, \dots, x_N\}$ denotes a point in the phase, i.e. it correspond to a instantaneous positions of N particles, each point $x_i \in (0, L)$.

17.1 Metropolis algorithm

Metropolis algorithm is used in order to implement the calculation of the system properties. A Markov chain is generated as a sequence of M points in N -dimensional phase space, $R = \{x_1, \dots, x_N\}$ where N is the number of dipoles. In each iteration, position of a single dipole with index i is displaced by $x'_i \rightarrow x_i + \xi_i$ where ξ_i is uniformly distributed random value in $(-\Delta t, \Delta t)$ range. The periodic boundary conditions (pbc)¹ are applied. and will be represented by $x'_i = pbc(x_i + \xi_i)$. The probability distribution in a quantum system corresponds to the square of the absolute value of the wave function 5, i.e.

$$p(x_1, \dots, x_N) = |(x_1, \dots, x_N)|^2 \quad (1)$$

¹If the value passes the upper bound returns to the beginning, and for the lower bound goes to the end

For a wave function written in a Jastrow pair product form it is written as

$$p(x_1, \dots, x_N) = |\Psi(x_1, \dots, x_N)|^2 \quad (2)$$

One needs to evaluate how the probability is changed in the move from the old to the new position. If the probability is increased, i.e. $p(x_1, \dots, x'_i, \dots, x_N) > p(x_1, \dots, x_i, \dots, x_N)$, then the move is always accepted. In the opposite case, it is accepted with the probability, $0 < p(x_1, \dots, x'_i, \dots, x_N)/p(x_1, \dots, x_i, \dots, x_N) < 1$. A practical way to do is to calculate the weight

$$w = \frac{p(x_1, \dots, x'_i, \dots, x_N)}{p(x_1, \dots, x_i, \dots, x_N)} \quad (3)$$

and compare it to a random value $\xi \in (0, 1)$. If $w > \xi$, the move is accepted, and the position in the phase space is changed $R_{i+1} = \{x_1, \dots, x'_i, \dots, x_N\}$. In the opposite case, the move is rejected, and the previous position in the phase space is conserved $R_{i+1} = \{x_1, \dots, x_i, \dots, x_N\}$.

After the dipole with index i was considered, we passed to the next index, until all dipoles were moved. A single step of the iteration corresponds to moving all N dipoles. All together M iterations are done.

Once the process is equilibrated, we sample the system properties such as the energy E , pair distribution function $g_2(x)$, etc. In particular $g_2(x)$ is calculated as a histogram of distances between particles on each iteration. Once the run is finished, I normalize the histogram and save the results obtained.

17.2 Expressions for energy calculation

During this research lots of formulas will be used for obtaining some results, in this case, as we are working on a 1-D gas, D (dimension) = 1, something that will simplify a lot of the formulas. These are the formulas that will be used:

- $\Delta u = u(R') - u(R)$, which represents the difference between the result of the current distribution of particles and the new one, when applying the u function.
- Drift force: $F_i = \sum_{j \neq i} u'_2(x_{ij}) \frac{x_i - x_j}{|x_i - x_j|}$ $F_j = \sum_{i \neq j} -u'_2(x_{ij}) \frac{x_i - x_j}{|x_i - x_j|}$, the force that each particle receives from the other particles.
- Kinetic energy (1) $E_{KIN}^{(1)} = -\frac{\hbar^2}{2m} \left[\sum_{i=1}^N F_i^2 + 2 \sum_{i < j} u''_2(r_{ij}) \right]$, that has in account the drift force and the interaction potential.
- Kinetic energy (2) $E_{KIN}^{(2)} = \frac{\hbar^2}{2m} \left[\sum_{i=1}^N F_i^2 \right]$, which only takes in account the drift force.

18 Tests

18.1 Ideal Fermi gas

It is useful to verify if the code works correctly. A good check for that it to reproduce the properties of an ideal Fermi gas. That is the model chosen for the comparison consists of N ideal Fermions in one dimension.

18.1.1 Model Hamiltonian

This model has a Hamiltonian which represents the total energy of the system, here the model consists in N atoms interacting via a known potential $V_{int}(x)$ of mass m . The Hamiltonian is computed with the kinetic energy and the interaction energy: $H = -E_{KIN}^{(2)} + \sum_{i<j}^N V_{int}(x_i - x_j)$

18.1.2 Exact wave function

Pauli exclusion principle[13] applies to fermions and prohibits any two fermions to be in the same position. The ground-state wave function is given by a Slater determinant

$$\Psi(x_1, \dots, x_N) = \det |\phi_{kl}(x_l)| \quad (4)$$

constructed from plane waves $\phi_{kl} = \exp(ikx_l)$ [18] where k is the set of allowed momenta. In one dimension, the Slater determinant (4) has a form of a Vandermonde determinant and it can be evaluated, resulting in a more simple expression

$$\Psi(x_1, \dots, x_N) = \prod_{i<j}^N \sin \frac{\Pi(x_i - x_j)}{L} \quad (5)$$

It is simpler in the sense that instead of N^3 operations required to evaluate a determinant, only N^2 operations are needed. In other words, the ground-state wave function can be cast in the Bijl-Jastrow pair-product form [1]

$$\Psi(x_1, \dots, x_N) = \prod_{i<j}^N f_2(x) \quad (6)$$

Another peculiarity of one dimension is that the wave function of N impenetrable bosonic atoms Ψ_B , i.e. hard spheres of zero diameter, is simply related to the wave function of ideal fermions, Ψ_F , Eq. (4) according to $\Psi_B = |\Psi_F|$ [7].

Applying this to our system, Girardeau's mapping means that the dipoles with Bose-Einstein and Fermi-Dirac statistics will have the same energy and pair distribution function.

18.1.3 Pair distribution function

The pair distribution function, $g_2(x)$, quantifies the probability of finding two particles separated by distance x . Its value can be numerically calculated by accumulating the histogram of distances between particles. The pair distribution function of an ideal Fermi gas is can be written explicitly as

$$g_2(x) = 1 - \left[\frac{\sin(\pi n x)}{\pi n x} \right]^2 \quad (7)$$

Equation (7) is very useful for the verification of the correctness of the implementation of the code and the consistency of the Metropolis algorithm.

18.1.4 Energy

As well, the energy can be compared with its exact value of the ideal Fermi gas

$$\frac{E}{N} = \frac{\pi^2 \hbar^2 n^2}{6m} \left(1 - \frac{1}{N^2}\right) \quad (8)$$

In Fig. 12 we compare the numerical result with the exact pair distribution function. We find a very good agreement, so we can conclude that the method is working correctly.

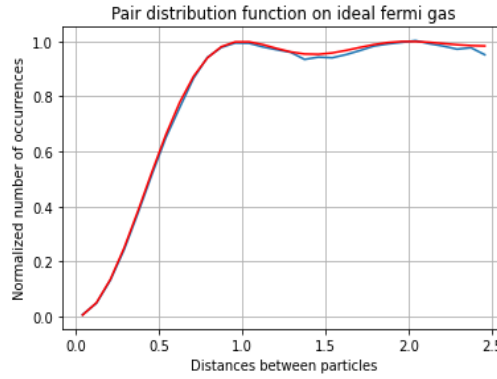


Figure 12: Pair distribution function of an ideal Fermi gas. Red line shows the exact analytic expression Eq. (7), blue line shows the numerical result obtained via Metropolis algorithm

In figure 13 we plot the relation between the energy per particle of the system with the density, which as it is shown, increases proportionally to the density, as it should be. Moreover, we can observe the relation with the energy per particle in relation with the reverse of the number of particles, as in figure 14, we can notice that in this case the bigger the number of particles, the lower the energy per particle is.

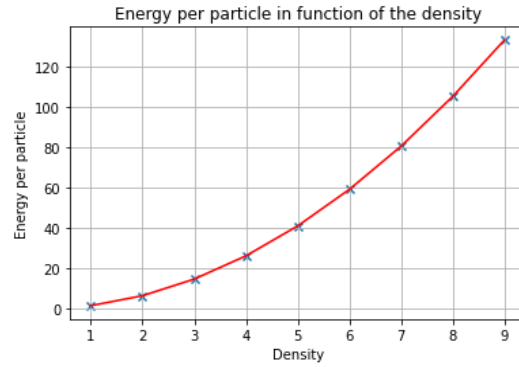


Figure 13: Energy per particle in function of the density of an ideal Fermi gas

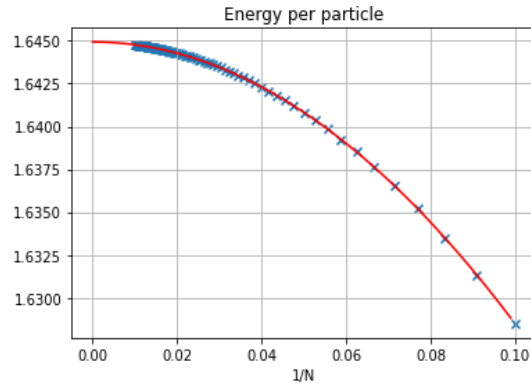


Figure 14: Energy per particle in function of the number of particles of an ideal Fermi gas

Here, in figure 15, we can see the plot of the kinetic energy per particle in function of the iteration of the process. The average value obtained is $E/N = 1.6408\hbar^2 n^2/m$ per particle. It can be remarked that the values are nearly the same on all iterations.

Meanwhile, in figure 16, we can see the plot of the energy of the drift force per particle in function of the iteration. The average value obtained is $E/N = 1.5567\hbar^2 n^2/m$ per particle. The statistical error can be approximated as σ/\sqrt{M} where the mean-square variance is $\sigma^2 = (1/M) \sum_{i=1}^M (E(i) - E)^2 = 0.21296$ which shows us that has a bit of statistical error.

As we can see, both values are similar as they should be, if the number of iterations was endless both values would be exactly the same, which can be described by $\pi^2 n^2/6 = 1.65$ for an infinite number of particles.

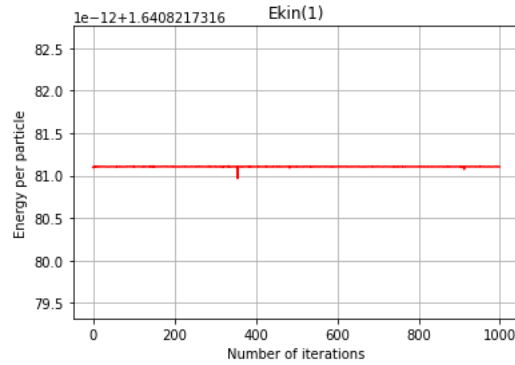


Figure 15: Kinetic energy obtained with 20 particles **change limits of the vertical axis to [0, 2]**

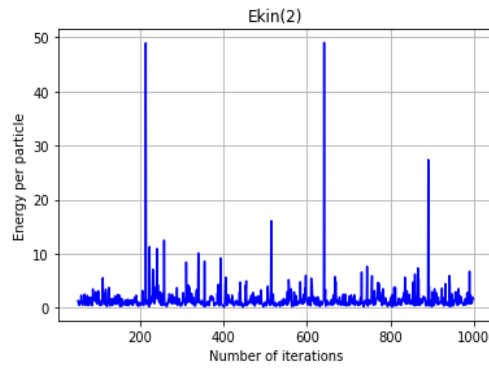


Figure 16: Drift force obtained with 20 particles

18.2 Purely dipolar system

Now it has been proven the correctness of the code we will reproduce the model of the real experiment. This also has an external potential which is an harmonic oscillator.

18.2.1 Model Hamiltonian

The Hamiltonian of this model is formed by the kinetic energy, the external potential, and the interaction energy: $H = E_{KIN}^{(1)} + \sum_{i < j}^N V_{int}(x_i - x_j)$

18.2.2 Trial wave function

To obtain the wave function a multidimensional integral must be done. However, using the Variational Monte-Carlo method it can be calculated too. One trial wave function must be chosen to perform the calculation, this should contain the maximum of knowledge of the system as possible. This function will be similar to the one of the fermionic gas, now it will have the form of:

$$\Psi(x_1, \dots, x_N) = \prod_{i < j}^N U_2(x) \quad (9)$$

18.2.3 Optimization of the variational parameters

In figure 17 we can see an example of how the optimum alpha parameter is obtained in function of the density, as it shows, this plot represents the energy per particle of the system in function of alpha in the points near its minimum, in this case the value of the density is equal to 2, and has been done with 640000 iterations in order to reduce the statistical error, as we can see the energy has been calculated twice per alpha value to show us the error obtained, and as the values are very similar it belongs on the estimated error. This points have been used afterwards for doing a quadratic fit in order to obtain a 2nd grade equation, which could give us the optimal value of alpha for that density, this has been done for densities from 1 to 10 and with that we will get the value of the minimum alpha.

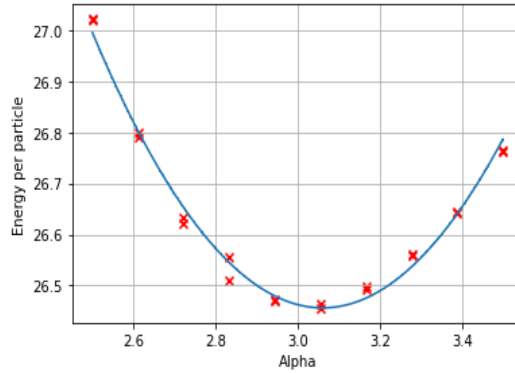


Figure 17: Energy per particle E/N dependence on the variational parameter α . The optimal value of the variational parameter α_{opt} corresponds to the minimum in the energy and is obtained by using a parabolic fit to the Monte Carlo data. Red symbols, Monte Carlo data. Blue line, parabolic fit.

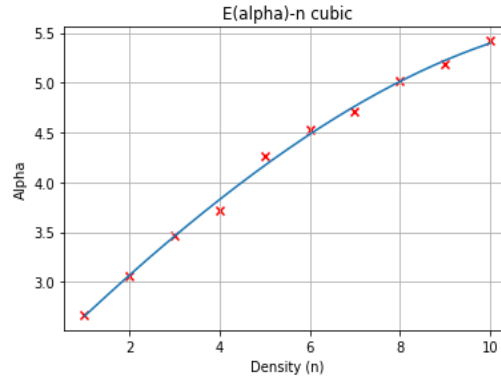


Figure 18: Dependence of the optimal value of the variational parameter α_{opt} on the linear density n . Cubic fitting of the equation of state for 20 particles. Red symbols, optimal values obtained as in Fig. 17. Blue line, cubic fit.

18.2.4 Potential energy

Finally, in figure 19 we can see the plot of the interaction potential energy, in which we can notice that in the plot there is a lot of variation between iterations. The average value is $E/N = 1.0486\hbar^2 n^2/m$ per particle, the statistical error can be approximated the same way as before, so the mean-squared variance is $\sigma^2 = (1/M) \sum_{i=1}^M (E(i) - E)^2 = 0.003247$ which is a value very narrow to zero.

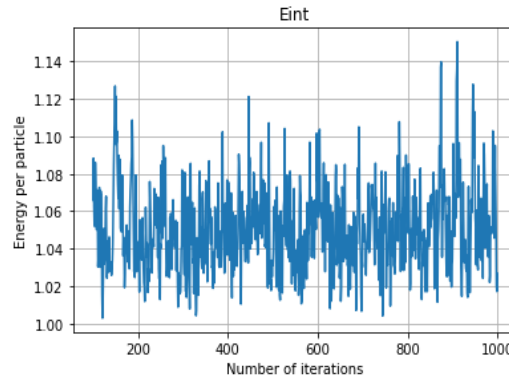


Figure 19: Interaction potential energy per particle obtained with 20 particles for $V(x) = 1/(x^2 + 1)$ interaction potential

18.2.5 Equation of state

Now, we are going to estimate the equation of state, in figure 20 we can see the values of the energy in terms of density, having fixed the optimum alpha, and with 3 different numbers of particles to show if there is any difference, for each value of N we have done a cubic fit to represent this equation, as we can see all the equations are very similar, there is a slightly difference between results, that indicates the more the number of particles the higher the energy per particle will be.

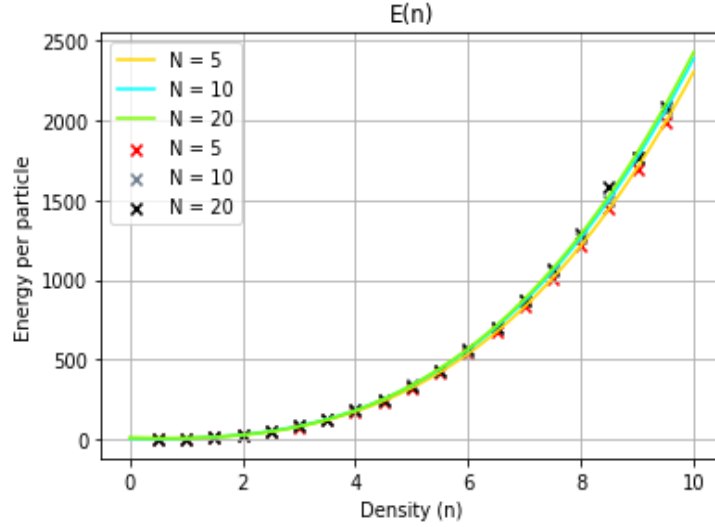


Figure 20: Ground-state energy per particle E/N for dipolar $1/|x|^3$ interaction potential as a function of the linear density nr_0 for different numbers of particles, $N = 5; 10; 20$.

19 Experimental system

19.1 Introduction

The full three-dimensional interactions consist of the short-range part, which can be approximated by a contact pseudopotential

$$U_{\text{contact}}(\mathbf{r}) = \frac{4\pi\hbar^2 a_{3D}}{m} \delta(\mathbf{r}) \frac{\partial}{\partial r}(r \cdot) \quad (10)$$

where a is the s -wave scattering length and m is the atomic mass, and the dipole-dipole potential[12]

$$U_{\text{dd}}(\mathbf{r}) = \frac{C_{\text{dd}}}{4\pi} \frac{(\mathbf{e}_1 \cdot \mathbf{e}_2) r^2 - 3(\mathbf{e}_1 \cdot \mathbf{r})(\mathbf{e}_2 \cdot \mathbf{r})}{r^5}. \quad (11)$$

where \mathbf{e}_1 and \mathbf{e}_2 are unit vectors showing orientation of the dipoles and \mathbf{r} the relative position. The coupling constant C_{dd} is $\mu_0\mu^2$ for particles having a permanent magnetic dipole moment μ (μ_0 is the permeability of vacuum).

We assume a quasi-one dimensional geometry with x being the longitudinal direction and yz being the transverse plane. In a very tight transverse confinement, the transverse density profile is given by the lowest state of a harmonic confinement

$$n(y, z) = \frac{1}{\pi a_{\text{ho}}^2} \exp\left(-\frac{y^2 + z^2}{a_{\text{ho}}^2}\right) \quad (12)$$

where $a_{\text{ho}} = \sqrt{\hbar/m\omega}$ is the harmonic oscillator length.

The effective 1D interaction is obtained by integrating out the yz degrees of freedom [6, 17] and contains two parts, the contact one

$$U_{\text{contact}}^{1D}(x) = -\frac{2\hbar^2}{ma_{1D}}\delta(x) \quad (13)$$

where $a_{1D} = -a_{\text{ho}}\left(\frac{a_{\text{ho}}}{a_{3D}} - C\right)$ is the one-dimensional s -wave scattering length with $C = |\zeta(1/2)|/\sqrt{2} \simeq 1.0326$ [16] and the dipolar part

$$U_{\text{dd}}^{1D}(x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_{\text{dd}}(x, y, z) n(y, z) dy dz \quad (14)$$

Here we assumed that the s -wave scattering length a_{3D} is of the same order as the oscillator length a_{ho} so that Confinement induced resonance is observed (otherwise one should use $C = 0$ instead of $C = 1.0326$). On the other hand we have assumed that the dipolar interactions are off resonant.

19.2 One-dimensional Hamiltonian

It can be shown [4, 5] that the resulting effective 1D Hamiltonian is

$$U_{\text{DDI}}^{1D}(u) = U_{dd}\tilde{V}_{dd}(u) \quad (15)$$

with the amplitude which depends on the orientation of the dipolar moment

$$U_{dd} = -\frac{1}{8} \left[1 + 3 \cos(2\theta) \right] \frac{d^2}{l_{\perp}^3} \quad (16)$$

and the dimensionless function

$$\tilde{V}_{dd}(u) = -2u + \sqrt{2\pi} (1 + u^2) e^{u^2/2} \text{erfc}(u/\sqrt{2}) \left] - \frac{8}{3}\delta(u) \quad (17)$$

The dipolar interaction potential results in a singular contribution represented by the δ - pseudopotential.

A possible way to fix the units is to consider

- l_{\perp} as the unit of length, is all distances are $u = x/l_{\perp}$
- $\hbar\omega_{\perp} = \hbar^2/(ml_{\perp}^2)$ as the unit of energy

The dimensionless Hamiltonian can be written as

$$\frac{\hat{H}}{\hbar\omega_{\perp}} = -\frac{1}{2} \sum_{i=1}^N \frac{\partial^2}{\partial u_i^2} + \sum_{i<j} (\tilde{U}_{dd} \tilde{V}_{dd}(u_{ij}) - \frac{2}{a/l_{\perp}} \delta(u_{ij})) \quad (18)$$

where $D = V(\theta)/(\hbar\omega_{\perp})$ is the dimensionless dipolar strength, a is the effective s -wave scattering length which contains two contributions, the short-range and the dipolar one.

There are three dimensionless parameters

- dipolar strength $\tilde{U}_{dd} = U_{dd}/(\hbar\omega_{\perp})$
- contact interaction strength, described by the dimensionless effective s -wave scattering length a/l_{\perp}
- linear density $nl_{\perp} = Nl_{\perp}/L$ where L is the system size

Note that in $D = 0$ case the only free dimensionless parameter is the gas parameter na or, equivalently, Lieb-Liniger parameter $\gamma = -2/na$.

The typical parameters are

- dipolar strength $\tilde{U}_{dd} = -0.407 \cdot \frac{1}{8} \left[1 + 3 \cos(2\theta) \right]$
- contact interaction strength, described by the dimensionless effective s -wave scattering length a/l_{\perp}
- linear density $nl_{\perp} = Nl_{\perp}/L$ where L is the system size

19.3 Experimental Parameters

??? **rewrite, if not it looks like you did the experiment** We used a 2D optical lattice to realize quasi-1D confinement. The lattice wavelength $\lambda = 741$ nm and the lattice depth is $30 E_{\text{R}}$, where $E_{\text{R}} = \hbar^2 k_{\text{R}}^2 / 2m$ and $k_{\text{R}} = 2\pi/\lambda$ is the lattice recoil energy and momentum, respectively. This trapping potential leads to a transverse trap frequency $\omega_{\perp} = 2\pi \times 24.58$ kHz and harmonic length $l_{\perp} = 952 a_0$, where a_0 is the Bohr radius. The atomic species we used for this work is ^{162}Dy , which has a mass of $161.9267984 m_a$ and a magnetic dipole moment of $9.93272 \mu_{\text{B}}$, where m_a is the atomic mass and μ_{B} is the Bohr magneton. The magnetic moment gives rise to a dipolar length of $129 a_0$, as defined in Eq. (3.2) of Ref. [12].

19.4 Experimental Data Explanation

The attached `excited_state_data.csv` file (see the Overleaf project source file folder) contains the necessary data to reproduce the latest version of Fig. 2 in Ref. [10]. Since we now account for the dipolar corrections to the Thomas-Fermi radii of the pre-load Bose-Einstein condensate, the lattice loading pattern and, by extension, the local density approximation (LDA) parameter $A^2 = N a_{1D}^2/a_{\parallel}^2$ (here a_{\parallel} is the harmonic length along the tubes) have been modified slightly versus the `arXiv` preprint. Below in Table 1, we summarize the column headings versus the terminologies used in the paper.

Column name	Note
<code>degree</code>	Dipole polarization in degrees.
<code>A^2</code>	The LDA parameter $A^2 = N a_{1D}^2/a_{\parallel}^2$. Here N is the central tube number, and a_{1D} is the 1D s -wave scattering length.
<code>A^2_err_lower</code>	Lower side of the uncertainty of the LDA parameter.
<code>A^2_err_upper</code>	Upper side of the uncertainty of the LDA parameter.
<code>a_1d</code>	1D s -wave scattering length in units of a_0 , computed with the single-atom (not using reduced mass) transverse harmonic length (i.e., $C = 1.0326$).
<code>R</code>	$R = \omega_B^2/\omega_D^2$, where ω_B and ω_D are the breathing the dipole mode frequencies, respectively.
<code>R_err</code>	Uncertainty of R .
<code>breathing_freq</code>	Breathing mode frequency in Hz.
<code>breathing_freq_err</code>	Uncertainty of breathing mode frequency in units of Hz.
<code>dipole_freq</code>	Dipole mode/Tube axial trap frequency in units of Hz.
<code>dipole_freq_err</code>	Uncertainty of dipole mode frequency in units of Hz.
<code>number_central</code>	Estimated atom number in the central tube.
<code>number_ensemble</code>	Estimated ensemble averaged atom number.

Table 1: Column heading explanation for Fig. 2 data.

Using the same procedure as in section 18.2.3, we will now proceed to calculate the optimal parameters α_{opt} , now taking into account the interaction potential as repulsive dipoles.

19.5 Breathing mode

In experiments, a trapped system is excited by changing slightly the frequency of the harmonic confinement ω_{ho} . This produces periodic oscillations of the size of the cloud known as a *breathing* mode. The frequency ω_b of such oscillations is measured and ratio ω_B^2/ω_D^2 is reported.

Equation of state can be locally approximated by a power law dependence, where

$$\mu = \frac{\partial E}{\partial N} = n \frac{\partial(E/N)}{\partial n} \quad (19)$$

is the chemical potential, C is the value of the chemical potential at the density n , a is the unit of length and γ is the polytropic index. The frequency of the breathing mode is then equal to

$$\frac{\omega_B^2}{\omega_D^2} = 2 + \gamma \quad (20)$$

The polytropic index can be found from the equation of state as

$$\gamma(n) = \frac{n}{\mu} \frac{\partial \mu}{\partial n} \quad (21)$$

For a cubic fit to the energy per particle

$$\frac{E}{N}(x) = C_0 + C_1x + C_2x^2 + C_3x^3 \quad (22)$$

where $x = nr_0$ is the dimensionless density. Then the chemical potential is given by

$$\mu(x) = C_1x + 2C_2x^2 + 3C_3x^3 \quad (23)$$

and the polytropic index becomes

$$\gamma(x) = \frac{C_1x + 2^2C_2x^2 + 3^2C_3x^3}{C_1x + 2C_2x^2 + 3C_3x^3} \quad (24)$$

In figure 22, we show the dependence of the energy per particle on the density, whereas in figure 23 we can see the chemical potential, obtained from the equation of state. Finally, we have the polytropic index which is shown in figure 24.

Similar as before, we can compute now the values with the interaction potential of dipoles, in figure 27, we can see the energy dependence on the density, whereas in figure 28 we can see the chemical potential, obtained from the equation of state. Finally, we have the polytropic index which is shown in figure 29.

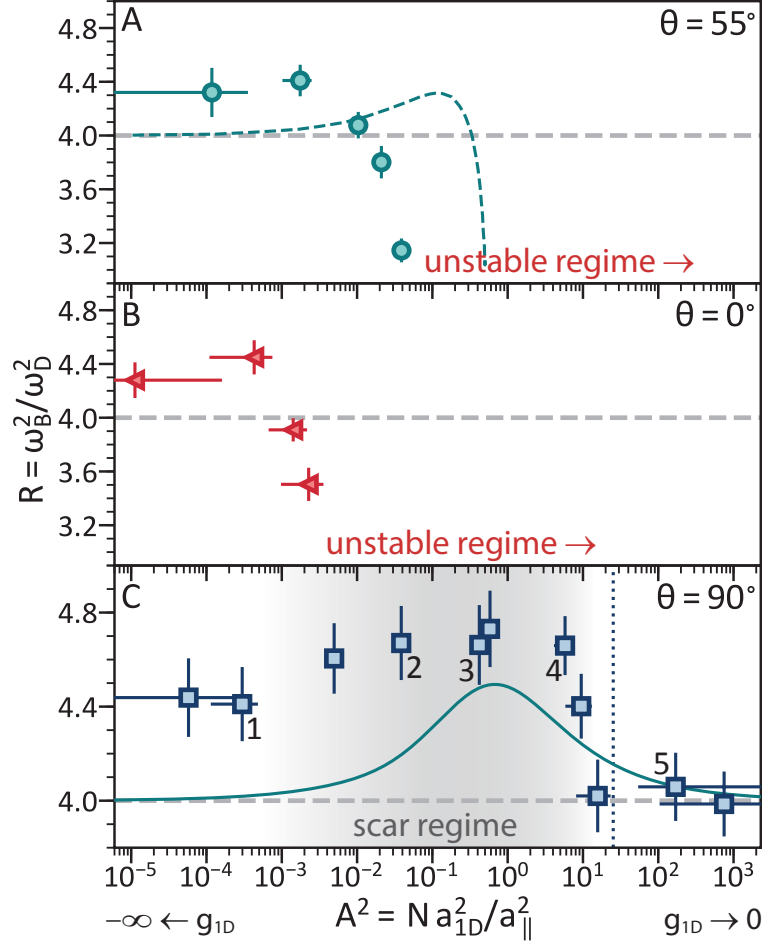


Figure 21: (taken from Ref [10], Fig. 2) Post-quench gas stiffness R versus interaction parameter A^2 in the attractive $g_{1D} < 0$ regime of the first holonomy cycle. Measurements are shown for the non dipolar ($\theta = 55^\circ$) and attractive DDI (0°) systems in panels A and B, respectively, and for the repulsive, 90° DDI-stabilized excited gas in panel C. In (A) and (B), an sTG gas exists in the unitary regime of $A^2 10^{-3}$. Beyond, however, the gas softens before collapsing near $A^2 \approx 10^{-1}$ and 10^{-2} , respectively. For comparison, the dashed green curve in panel A plots data from the non dipolar variational Monte Carlo simulation of Ref. [?]. (C) Surprisingly, the repulsive DDI system remains stable beyond the unitary regime. This allows scar states to emerge around intermediate coupling strengths, indicated in gray, before crossing over into the $R = 4$ weakly attractive, excited Bose gas regime beyond $A^2 \approx 10$. The solid curve is the Bethe ansatz prediction. The vertical dotted line indicates where the contact and the short-range 1D-regularized DDI contributions become approximately equal [?]. Numbers refer to points in Figs. ??B and ??. The error bars here and in subsequent figures represent the standard error.

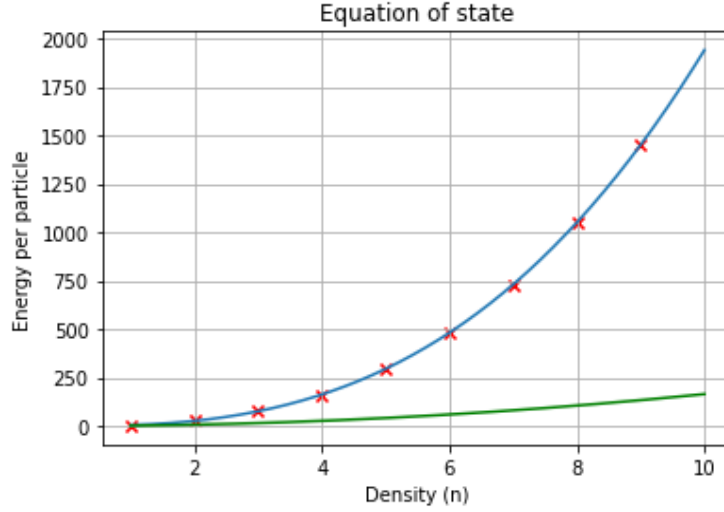


Figure 22: Energy per particle in a system with $V_{int} = 1/|x|^3$ interaction potential calculated with the optimal value of the variational parameter α as a function of the linear density for $N = 10$ particles. Red points, Monte Carlo results; blue line, polynomial fit (22), Green line, energy of the Ideal Fermi gas (8).

20 Conclusions

Once all the results have been obtained, we are at the point of doing comparisons between the numerical results and the experimental results.

As we can see in the C plot of figure 21, we can observe that the value obtained of the frequency of the breathing mode comprise between 4 and 4.5, if we compare it with the plot obtained via variational Monte Carlo method in figure 30, which also uses $\theta = 90^\circ$ we can notice that both values are in the range of 4 near 0, differing in the scar regime where it increases the value in the experimental result, this is due that in the experiment is considered the short range interaction apart from the purely dipolar interaction, but this short range interaction is not considered on this work, so the difference between both results is due to this.

Overall, the code has worked properly when doing new things, but in some cases some problems appeared, so it was useful doing a planning adding some hours in case of something happened, also at the beginning of the implementation of the code, the code could be proved that worked correctly, but after that was more difficult to prove the correctness, as no theoretical results were available, but finally, the numerical result in comparison with the experiment was similar, so we can conclude that it was a successful project.

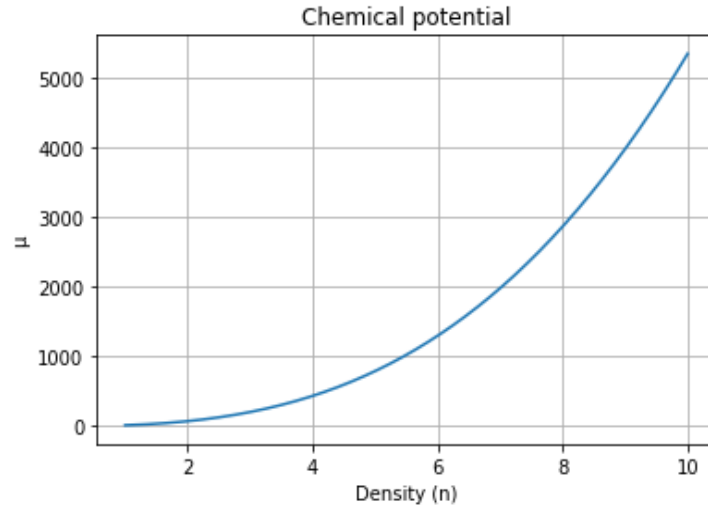


Figure 23: Chemical potential in a system with $V_{int} = 1/|x|^3$ interaction potential calculated with the optimal value of the variational parameter α as a function of the linear density for $N = 10$ particles (23).

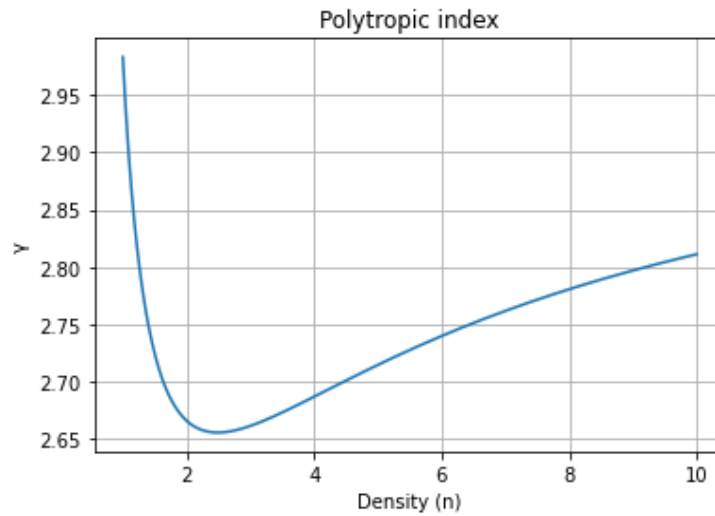


Figure 24: Polytropic index in a system with $V_{int} = 1/|x|^3$ interaction potential calculated with the optimal value of the variational parameter α as a function of the linear density for $N = 10$ particles (24).

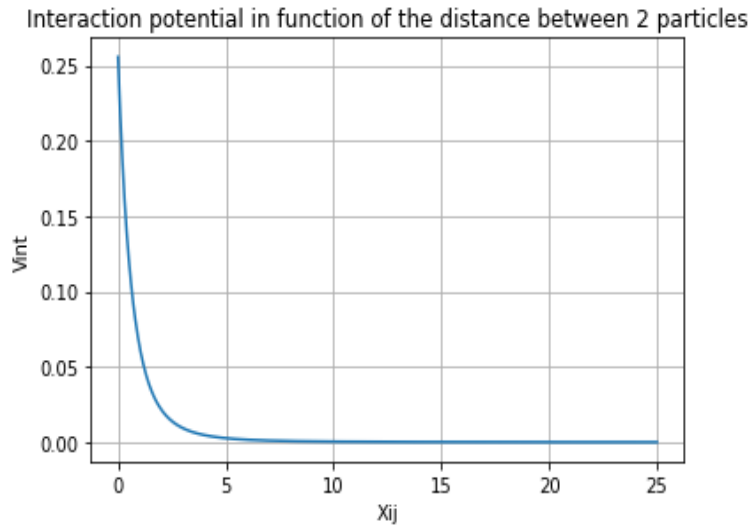


Figure 25: Interaction potential, corresponding to the dipolar interactions in experiment[10], $V_{int} = V_{dd}(x) \cdot U_{dd}$.

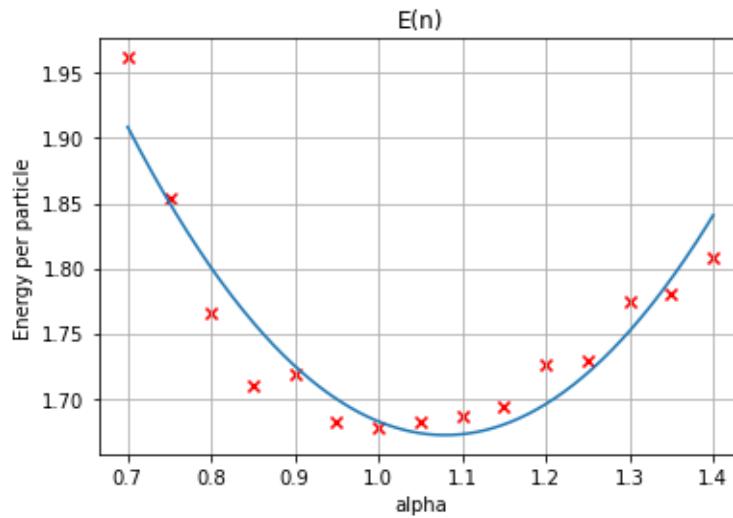


Figure 26: Typical example of the dependence of the variational energy on the variational parameter α for the experimentally relevant interaction potential $V_{int} = V_{dd}(x) \cdot U_{dd}$. The optimal value of the variational parameter α corresponds to the minimum.

Red symbols, variational Monte Carlo data;
Blue line, the result of the parabolic fit.

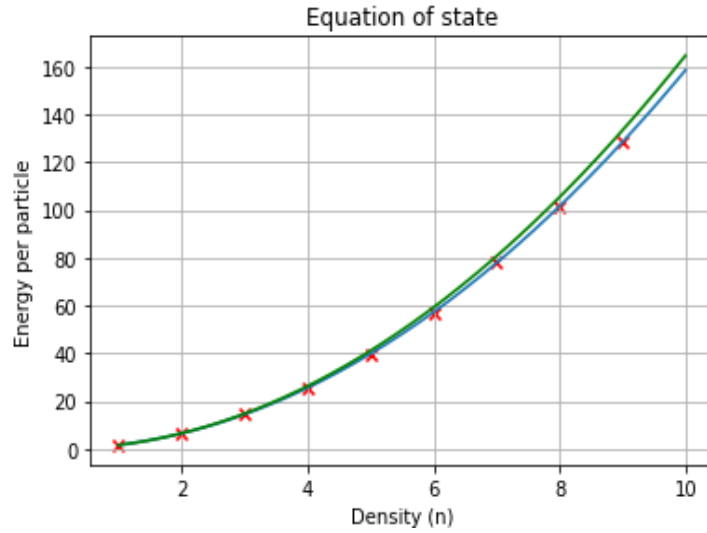


Figure 27: Equation of state of the system with $V_{int} = V_{dd}(x) \cdot U_{dd}$ with the optimum alpha for each density. Red points, Monte Carlo results; Blue line, polynomial fit (22), Green line, energy of the Ideal Fermi gas (8).

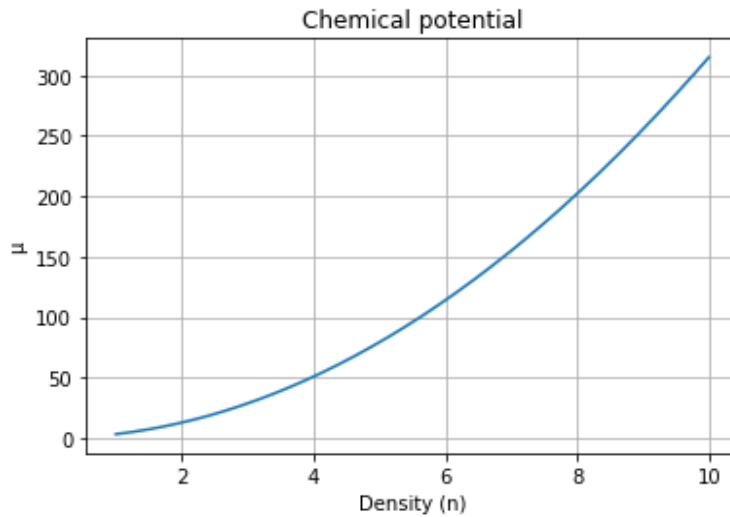


Figure 28: Chemical potential of the system with $V_{int} = V_{dd}(x) \cdot U_{dd}$ (23).

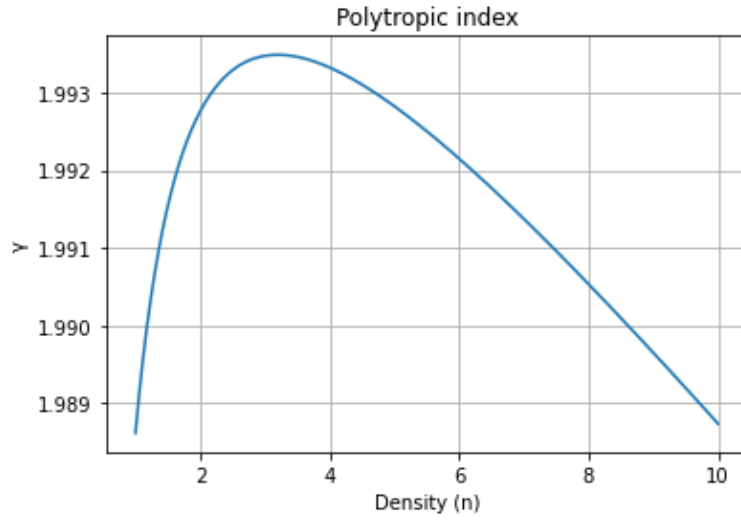


Figure 29: Polytropic index of the system for $V_{int} = V_{dd}(x) \cdot U_{dd}$ (24).

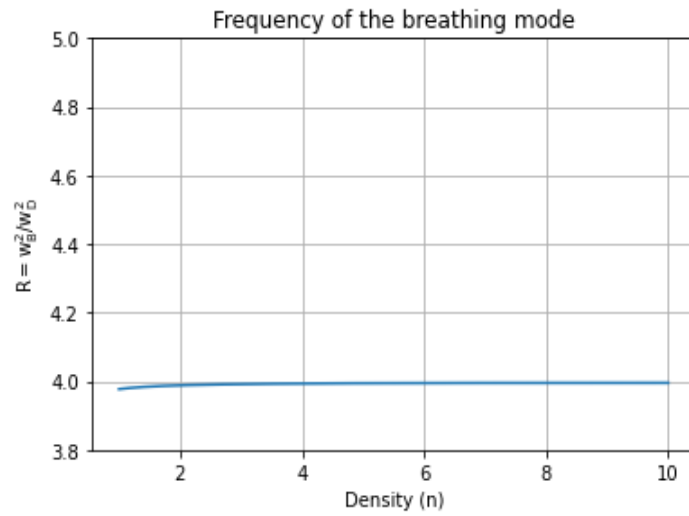


Figure 30: Frequency of the breathing mode of the system for $V_{int} = V_{dd}(x) \cdot U_{dd}$ in function of the density (20).

21 Bibliography

References

- [1] Bijl-jastrow wave function.
- [2] Salaries website of jobs near your zone.
- [3] Max Born. Zur quantenmechanik der stovorgnge. *Zeitschrift fr Physik*, 37(12):863–867, December 1926.
- [4] F. Deuretzbacher, J. C. Cremon, and S. M. Reimann. Ground-state properties of few dipolar bosons in a quasi-one-dimensional harmonic trap. *Phys. Rev. A*, 81:063616, Jun 2010.
- [5] F. Deuretzbacher, J. C. Cremon, and S. M. Reimann. Erratum: Ground-state properties of few dipolar bosons in a quasi-one-dimensional harmonic trap [phys. rev. a 81, 063616 (2010)]. *Phys. Rev. A*, 87:039903, Mar 2013.
- [6] W I Friesen and B Bergersen. Dielectric response of a one-dimensional electron gas. *Journal of Physics C: Solid State Physics*, 13(36):6627–6640, dec 1980.
- [7] M. Girardeau. Relationship between systems of impenetrable bosons and fermions in one dimension. *Journal of Mathematical Physics*, 1(6):516–523, November 1960.
- [8] Xi-Wen Guan, Murray T. Batchelor, and Chaohong Lee. Fermi gases in one dimension: From bethe ansatz to experiments. *Reviews of Modern Physics*, 85(4):1633–1691, November 2013.
- [9] Wil Kao, Kuan-Yu Li, Kuan-Yu Lin, Sarang Gopalakrishnan, and Benjamin L. Lev. Creating quantum many-body scars through topological pumping of a 1d dipolar gas, 2020.
- [10] Wil Kao, Kuan-Yu Li, Kuan-Yu Lin, Sarang Gopalakrishnan, and Benjamin L. Lev. Topological pumping of a 1d dipolar gas into strongly correlated prethermal states. *Science*, 371(6526):296–300, January 2021.
- [11] T. Kinoshita. Observation of a one-dimensional tonks-girardeau gas. *Science*, 305(5687):1125–1128, August 2004.
- [12] T Lahaye, C Menotti, L Santos, M Lewenstein, and T Pfau. The physics of dipolar bosonic quantum gases. *Reports on Progress in Physics*, 72(12):126401, nov 2009.
- [13] Irving Langmuir. THE ARRANGEMENT OF ELECTRONS IN ATOMS AND MOLECULES. *Journal of the American Chemical Society*, 41(6):868–934, June 1919.

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- [14] Renate Meyer, Bo Cai, and François Perron. Adaptive rejection metropolis sampling using lagrange interpolation polynomials of degree 2. *Computational Statistics & Data Analysis*, 52(7):3408–3423, March 2008.
 - [15] Ronald Newburgh, Joseph Peidle, and Wolfgang Rueckner. Einstein, perlin, and the reality of atoms: 1905 revisited. *American Journal of Physics*, 74(6):478–481, June 2006.
 - [16] M. Olshanii. Atomic scattering in the presence of an external confinement and a gas of impenetrable bosons. *Phys. Rev. Lett.*, 81:938, 1998.
 - [17] Luke Shulenburger, Michele Casula, Gaetano Senatore, and Richard M. Martin. Correlation effects in quasi-one-dimensional quantum wires. *Phys. Rev. B*, 78:165303, Oct 2008.
 - [18] J. C. Slater. The theory of complex spectra. *Physical Review*, 34(10):1293–1322, November 1929.