Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.

- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.

- Include the source code of your program. Comment your program properly.

- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.

- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.

- Try to evaluate the reliabilty and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.

- Try to give an interpretation of you results in your answers to the problems.

- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.

- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.

Format for electronic delivery of report and programs

The preferred format for the report is a PDF file. You can also use DOC or postscript formats. As programming language we prefer that you choose between C/C++ and Fortran90/95. You could also use Java or Python as programming languages. Matlab/Maple/Mathematica/IDL are not accepted, but you can use them to check your results where possible. Finally, we do prefer that you work together. Optimal working groups consist of 2-3 students, but more people can collaborate. You can then hand in a common report.

Project 2, Variational Monte Carlo for BEC with ^{87}Rb, deadline april 16 12am (midnight)

The spectacular demonstration of Bose-Einstein condensation (BEC) in gases of alkali atoms ^{87}Rb, ^{23}Na, ^{7}Li confined in magnetic traps [1, 2, 3] has led to an explosion of interest in confined Bose systems. Of interest is the fraction of condensed atoms, the nature of the condensate, the excitations above the condensate, the atomic density in the trap as a function of Temperature and the critical temperature of BEC, T_c. The extensive progress made up to early 1999 is reviewed by Dalfovo et al.[4].

A key feature of the trapped alkali and atomic hydrogen systems is that they are dilute. The characteristic dimensions of a typical trap for ^{87}Rb is $a_{h0} = (\hbar/m\omega_\perp)^{\frac{1}{2}} = 1 - 2 \times 10^4$ Å (Ref. [1]). The interaction between ^{87}Rb atoms can be well represented by its s-wave scattering length, a_{Rb}. This scattering length lies in the range $85 < a_{Rb} < 140a_0$ where $a_0 = 0.5292$ Å is the Bohr radius. The definite value $a_{Rb} = 100a_0$ is usually selected and for calculations the definite ratio of atom size to trap size $a_{Rb}/a_{h0} = 4.33 \times 10^{-3}$ is usually chosen [4]. A typical ^{87}Rb atom density in the trap is $n \simeq 10^{12} - 10^{14}$ atoms/cm^3 giving an inter-atom spacing $\ell \simeq 10^4$ Å. Thus the effective atom size is small compared to both the trap size and the inter-atom spacing, the condition for diluteness (i.e., $na_{Rb}^3 \simeq 10^{-6}$ where $n = N/V$ is the number density). In this limit, although the interaction is important, dilute gas approximations such as the Bogoliubov theory [5], valid for small na^3 and large condensate fraction $n_0 = N_0/N$, describe the system well. Also, since most of the atoms are in the condensate (except near T_c), the Gross-Pitaevskii equation [6, 7] for the condensate describes the whole gas well. Effects of atoms excited above the condensate have been incorporated within the Popov approximation [8].

The aim of this project is to use the Variational Monte Carlo (VMC) method and evaluate the ground state energy of a trapped, hard sphere Bose gas for different numbers of particles with a specific trial wave function. See Ref. [9] for a discussion of VMC.

This wave function is used to study the sensitivity of condensate and non-condensate properties to the hard sphere radius and the number of particles. The trap we will use is a spherical (S) or an elliptical (E) harmonic trap in three dimensions given by

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega_{ho}^2 r^2 & (S) \\ \frac{1}{2}m[\omega_{ho}^2(x^2 + y^2) + \omega_z^2 z^2] & (E) \end{cases} \qquad (1)$$

where (S) stands for symmetric and

$$H = \sum_i^N \left(\frac{-\hbar^2}{2m}\nabla_i^2 + V_{ext}(\mathbf{r}_i) \right) + \sum_{i<j}^N V_{int}(\mathbf{r}_i, \mathbf{r}_j), \qquad (2)$$

as the two-body Hamiltonian of the system. Here ω_{ho}^2 defines the trap potential strength. In the case of the elliptical trap, $V_{ext}(x, y, z)$, $\omega_{ho} = \omega_\perp$ is the trap frequency in the perpendicular or xy plane and ω_z the frequency in the z direction. The mean square vibrational amplitude of a single boson at $T = 0K$ in the trap (1) is $< x^2 >= (\hbar/2m\omega_{ho})$ so that

$a_{ho} \equiv (\hbar/m\omega_{ho})^{\frac{1}{2}}$ defines the characteristic length of the trap. The ratio of the frequencies is denoted $\lambda = \omega_z/\omega_\perp$ leading to a ratio of the trap lengths $(a_\perp/a_z) = (\omega_z/\omega_\perp)^{\frac{1}{2}} = \sqrt{\lambda}$.

We represent the inter boson interaction by a pairwise, hard core potential

$$V_{int}(|\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases} \tag{3}$$

where a is the hard core diameter of the bosons. Clearly, $V_{int}(|\mathbf{r}_i - \mathbf{r}_j|)$ is zero if the bosons are separated by a distance $|\mathbf{r}_i - \mathbf{r}_j|$ greater than a but infinite if they attempt to come within a distance $|\mathbf{r}_i - \mathbf{r}_j| \leq a$.

Our trial wave function for the ground state with N atoms is given by

$$\Psi_T(\mathbf{R}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N, \alpha, \beta) = \prod_i g(\alpha, \beta, \mathbf{r}_i) \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|), \tag{4}$$

where α and β are variational parameters. The single-particle wave function is proportional to the harmonic oscillator function for the ground state, i.e.,

$$g(\alpha, \beta, \mathbf{r}_i) = \exp\left[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right]. \tag{5}$$

For spherical traps we have $\beta = 1$ and for non-interacting bosons ($a = 0$) we have $\alpha = 1/2a_{ho}^2$. The correlation wave function is

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \tag{6}$$

Exercise 1: Variational Monte Carlo study of the BEC ground state

1a) Find analytic expressions for the local energy

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} H \Psi_T(\mathbf{R}), \tag{7}$$

for the above trial wave function of Eq. (4). Compute also the analytic expression for the drift force to be used in importance sampling

$$F = \frac{2\nabla\Psi_T}{\Psi_T}. \tag{8}$$

1b) Write a Variational Monte Carlo program which uses standard Metropolis sampling and compute the ground state energy of a spherical harmonic oscillator ($\beta = 1$) with no interaction. Use natural units and make an analysis of your calculations using both the analytic expression for the local energy and a numerical calculation of the kinetic energy using numerical derivation. Compare the CPU time difference. You should also parallelize your code. The only variational parameter is α. Perform these calculations for $N = 10$, 100 and 500 atoms. Compare your results with the exact answer.

1c) We turn now to the elliptic trap with a hard core interaction. We fix, as in Refs. [10, 11] $a/a_{ho} = 0.0043$. Introduce lengths in units of a_{ho}, $r \to r/a_{ho}$ and energy in units of $\hbar\omega_{ho}$. Show then that the original Hamiltonian can be rewritten as

$$H = \sum_{i=1}^{N} \frac{1}{2}\left(-\nabla_i^2 + x_i^2 + y_i^2 + \gamma^2 z_i^2\right) + \sum_{i<j} V_{int}(|\mathbf{r}_i - \mathbf{r}_j|). \qquad (9)$$

What is the expression for γ? Choose the initial value for $\beta = \gamma = 2.82843$ and set up a VMC program which computes the ground state energy using the trial wave function of Eq. (4). using only α as variational parameter. Use standard Metropolis sampling and vary the parameter α in order to find a minimum. Perform the calculations for $N = 10, 50$ and $N = 100$ and compare your results to those from the ideal case in the previous exercise.

1d) We repeat exercise 1c), but now we replace the brute force Metropolis algorithm with importance sampling based on the Fokker-Planck and the Langevin equations. Discuss your results and comment on eventual differences between importance sampling and brute force sampling.

In the statistical analysis of your results you should use for example the blocking technique from Project 1. Your code should reproduce the results of Refs. [10, 11].

Literature

References

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