University of Oslo
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Computational physics II: Quantum mechanical systems

Project 1

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1 Introduction

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. This trial wave function is used to study the sensitivity of condensate and non-condensate properties to the hard sphere radius and the number of particles.

2 Theory

The trap we will use is a spherical (S) or an elliptical (E) harmonic trap in one, two and finally three dimensions, with the latter given by

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

The Hamiltonian of the system will be

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

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 $\langle x^2\rangle = (\hbar/2m\omega_{ho})$ 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 $(a_\perp/a_z) = (\omega_z/\omega_\perp)^{\frac{1}{2}} = \sqrt{\lambda}$.

Note: In the rest of this report, as well as in accompanying source code, we will use natural units with $\hbar = m = 1$.

We will represent the inter-boson interaction by a pairwise, repulsive potential:

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

where a is the so-called 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 $|\mathbf{r}_i - \mathbf{r}_j| \le a$.

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

$$\begin{aligned}\Psi_T(\mathbf{r}) &= \Psi_T(\mathbf{r}_1,\mathbf{r}_2,\dots\mathbf{r}_N,\alpha,\beta) \\ &= \prod_i g(\alpha,\beta,\mathbf{r}_i)\prod_{i<j} f(a,|\mathbf{r}_i-\mathbf{r}_j|), \end{aligned} \quad (4)$$

where α and β are variational parameters. We choose the single-particle wave function to be proportional to the harmonic oscillator function for the ground state, i.e., we define $g(\alpha,\beta,\mathbf{r}_i)$ as:

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

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

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

2.1 Defining the Objective

We wish to evaluate the expectation value of the Hamiltonian. We cannot do this without the true wavefunction of the system, something we do not possess. We can, however, approximate the energy with the trial wavefunction.

$$E[H] = \langle H \rangle = \frac{\int \mathrm{d}\boldsymbol{R}\, \Psi_T^* H \Psi_T}{\int \Psi_T^* \Psi_T}. \quad (7)$$

where $\boldsymbol{R}$ is the matrix containing all the positions of the particles in the system, $\boldsymbol{R} = [\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N]$. In order to numerically evaluate this integral we first manipulate it a bit. The probability density at position $\boldsymbol{R}$, under the trial wavefunction, is

$$P(\boldsymbol{R}, \boldsymbol{\alpha}) = \frac{|\Psi_T|^2}{\int \mathrm{d}\boldsymbol{R}\, |\Psi_T|^2}. \quad (8)$$

where $\boldsymbol{\alpha}$ is used for shorthand and represents the vector of all the variational parameters. We finally define a new quantity, called the local energy:

$$E_L(\boldsymbol{R}, \boldsymbol{\alpha}) = \frac{1}{\Psi_T} H \Psi_T \quad (9)$$

Combining these two definitions we can now rewrite $\langle H \rangle$ as follows:

$$\begin{aligned} \langle H \rangle &= \int \mathrm{d}\boldsymbol{R}\, P(\boldsymbol{R}, \boldsymbol{\alpha}) E_L(\boldsymbol{R}, \boldsymbol{\alpha}) \\ &\approx \frac{1}{N} \sum_{i=1}^{N} E_L(\boldsymbol{R}_i, \boldsymbol{\alpha}), \end{aligned} \quad (10)$$

where R_i are randomly drawn positions from the PDF $P(\boldsymbol{R}, \boldsymbol{\alpha})$. We have therefore that estimating the average value of E_L yields an approximated value for $\langle H \rangle$. This value is in turn be an upper bound on the ground state energy, E_0. By the variational principle, if we minimize $\langle H \rangle$ under the variational parameters, we find an estimate for the true ground state energy of the system.

2.2 Finding an Analytical Expression for E_L

As the local energy will is the quantity we are interested in computing for a large set of positions we would do well to consider how best to evaluate this expression effectively. Straight forward numerical derivation is of course an option, but this is likely to be quite time-expensive to do.

The hard part of the expression for E_L is

$$\frac{1}{\Psi_L} \sum_{k}^{N} \nabla_k^2 \Psi_L. \quad (11)$$

To get going, we rewrite the wavefunction as

$$\Psi_L(\boldsymbol{R}) = \prod_i \phi(\boldsymbol{r}_i) \exp\left(\sum_{i<j} u(r_{ij}) \right), \quad (12)$$

where $r_{ij} = \|\boldsymbol{r}_{ij}\| = \|\boldsymbol{r}_i - \boldsymbol{r}_j\|$, $u(r_{ij}) = \ln f(r_{ij})$, and $\phi(\boldsymbol{r}_i) = g(\alpha, \beta, \boldsymbol{r}_i)$.

Lets first evaluate the gradient with respect to particle k

$$\begin{aligned} \boldsymbol{\nabla}_k \Psi_T(\boldsymbol{r}) &= \boldsymbol{\nabla}_k \prod_i \phi(\boldsymbol{r}_i) \exp\left(\sum_{i<j} u(r_{ij}) \right) \\ &= \prod_{i \neq k} \phi(\boldsymbol{r}_i) \exp\left(\sum_{i<j} u(r_{ij}) \right) \boldsymbol{\nabla}_k \phi(\boldsymbol{r}_k) \\ &+ \prod_i \phi(\boldsymbol{r}_i) \boldsymbol{\nabla}_k \exp\left(\sum_{i<j} u(r_{ij}) \right) \\ &= \Psi_T \left[\frac{\boldsymbol{\nabla}_k \phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)} + \sum_{j \neq k} \boldsymbol{\nabla}_k u(r_{kj}) \right]. \end{aligned} \quad (13)$$

The first term is evaluated quite simply:

$$\begin{aligned}\frac{\boldsymbol{\nabla}_k\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)} &= \frac{\boldsymbol{\nabla}_k}{\phi(\boldsymbol{r})}\exp\left[-\alpha\left(x_k^2+y_k^2+\beta z_k^2\right)\right]\\ &= \frac{\boldsymbol{\nabla}_k}{\phi(\boldsymbol{r})}\exp\left[-\alpha\hat{\boldsymbol{r}}_k^2\right]\\ &= -2\alpha\hat{\boldsymbol{r}}_k,\end{aligned} \tag{14}$$

where the notation $\hat{\boldsymbol{r}}_k = (x, y, \beta z)$ is introduced for brevity. Note that in the 1D and 2D case we simply have $\hat{\boldsymbol{r}}_k = \boldsymbol{r}_k$.

The second term may be evaluated as follows:

$$\begin{aligned}\boldsymbol{\nabla}_k u(r_{kj}) &= u'(r_{kj})\boldsymbol{\nabla}_k\sqrt{\|\boldsymbol{r}_k-\boldsymbol{r}_j\|^2}\\ &= \frac{u'(r_{kj})}{2r_{kj}}\boldsymbol{\nabla}_k\left(\|\boldsymbol{r}_k\|^2-2\boldsymbol{r}_k\cdot\boldsymbol{r}_j+\|r_j\|^2\right)\\ &= u'(r_{kj})\frac{\boldsymbol{r}_{kj}}{r_{kj}}\\ &= \frac{\partial}{\partial r_{kj}}\left[\ln\left(1-\frac{a}{r_{kj}}\right)\right]\frac{\boldsymbol{r}_{kj}}{r_{kj}}\\ &= \frac{\boldsymbol{r}_{kj}}{r_{kj}}\frac{a}{r_{kj}(r_{kj}-a)}.\end{aligned} \tag{15}$$

Now we can find the Laplacian by taking the divergence of (13)

$$\begin{aligned}\frac{1}{\Psi_L}\nabla_k^2\Psi_L &= \frac{1}{\Psi_L}\boldsymbol{\nabla}_k\cdot\Psi_T\left[\frac{\boldsymbol{\nabla}_k\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)}+\sum_{j\neq k}\boldsymbol{\nabla}u(r_{kj})\right]\\ &= \frac{\nabla_k^2\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)}+\sum_{j\neq k}\nabla_k^2u(r_{kj})\\ &+\frac{\boldsymbol{\nabla}_k(\phi(\boldsymbol{r}_k))\cdot\left(\sum_{j\neq k}\boldsymbol{\nabla}_k u(r_{kj})\right)}{\phi(\boldsymbol{r}_k)}\\ &+\left[\left(\frac{\boldsymbol{\nabla}_k\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)}+\sum_{j\neq k}\boldsymbol{\nabla}_k u(r_{kj})\right)\right.\\ &\left.\cdot\left(\sum_{j\neq k}\boldsymbol{\nabla}_k u(r_{kj})\right)\right]\\ &= \frac{\nabla_k^2\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)}+2\frac{\boldsymbol{\nabla}_k\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)}\cdot\sum_{j\neq k}\left(\frac{\boldsymbol{r}_{kj}}{r_{kj}}u'(r_{kj})\right)\\ &+\sum_{i,j\neq k}\frac{\boldsymbol{r}_{ki}\cdot\boldsymbol{r}_{kj}}{r_{ki}r_{kj}}u'(r_{ki})u'(r_{kj})+\sum_{j\neq k}\nabla_k^2u(r_{kj}).\end{aligned} \tag{16}$$

There are two new quantities here which need to be evaluated before we are done:

$$\frac{\nabla_k^2\phi(\boldsymbol{r}_k)}{\phi(\boldsymbol{r}_k)} = 2\alpha\left[2\alpha\|\hat{\boldsymbol{r}}_k\|^2-d(\beta)\right],$$
$$\text{with } d(\beta)=\begin{cases}1 & \text{for 1D}\\ 2 & \text{for 2D}\\ 2+\beta & \text{for 3D}\end{cases}, \tag{17}$$

and

$$\begin{aligned}\nabla_k^2u(r_{kj}) &= \boldsymbol{\nabla}_k\cdot u'(r_{kj})\frac{\boldsymbol{r}_{kj}}{r_{kj}}\\ &= u'(r_{kj})\frac{2}{r_{kj}}+\frac{\boldsymbol{r}_{kj}}{r_{kj}}\cdot\boldsymbol{\nabla}_k u'(r_{kj})\\ &= u''(r_{kj})+\frac{2}{r_{kj}}u'(r_{kj}),\end{aligned} \tag{18}$$

where

$$\begin{aligned}u''(r_{ij}) &= \frac{\partial^2}{\partial r_{ij}^2}\ln\left(1-\frac{a}{r_{ij}}\right)\\ &= \frac{a(a-2r_{ij})}{r_{ij}^2(r_{ij}-a)^2}.\end{aligned} \tag{19}$$

Inserting all of this back into (16) we get:

$$\begin{aligned}\frac{1}{\Psi_L}\nabla_k^2\Psi_L &= 2\alpha\Big[2\alpha\|\hat{\boldsymbol{r}}_k\|^2 - d(\beta)\Big] \\ &\quad - 4\alpha\hat{\boldsymbol{r}}_k \cdot \left[\sum_{j\neq k}\frac{\boldsymbol{r}_{kj}}{r_{kj}}\frac{a}{r_{kj}(r_{kj}-a)}\right] \\ &\quad + \sum_{i,j\neq k}\frac{\boldsymbol{r}_{ki}\cdot\boldsymbol{r}_{kj}}{r_{ki}r_{kj}}\frac{a}{r_{ki}(r_{ki}-a)}\frac{a}{r_{kj}(r_{kj}-a)} \\ &\quad + \sum_{j\neq k}\left(\frac{a(a-2r_{kj})}{r_{kj}^2(r_{kj}-a)^2} + \frac{2}{r_{kj}}\frac{a}{r_{kj}(r_{kj}-a)}\right).\end{aligned} \tag{20}$$

We may note that without interactions ($a = 0$), this simplifies to only the first term, as all the other terms are proportional to a.

The complete expression for the local energy is then:

$$\begin{aligned}E_L &= \frac{1}{\Psi_T}H\Psi_T \\ &= \sum_i V_{ext}(\boldsymbol{r}_i) + \sum_{i<j}V_{int}(\boldsymbol{r}_i,\boldsymbol{r}_j) - \frac{\hbar^2}{2m}\sum_k\frac{1}{\Psi_T}\nabla_k^2\Psi_T\end{aligned} \tag{21}$$

where we substitute in (20) in the final sum.

2.3 Finding an Analytical Expression for the Quantum Drift Force

Anticipating its later use, we will also find an expression for the so called quantum drift force, which we shall use when we consider importance sampling. For now, we just give its definition:

$$\boldsymbol{F}_k = \frac{2\boldsymbol{\nabla}_k\Psi_T}{\Psi_T} \tag{22}$$

This is interpreted as the force acting on particle k due to the trap and/or presence of other particles. Luckily this can now be quickly evaluated due to the results of the previous section,

$$\boldsymbol{F}_k = 2\left[\sum_{j\neq k}\frac{\boldsymbol{r}_{kj}}{r_{kj}}\frac{a}{r_{kj}(r_{kj}-a)} - 2\alpha\hat{\boldsymbol{r}}_k\right]. \tag{23}$$