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. 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

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

where (S) stands for symmetric and

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

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

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

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

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 $|\mathbf{r}_i-\mathbf{r}_j| \leq a$.

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

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

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.,

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

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

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

We wish to evaluate the expectation value of the Hamiltonian, which we can approximate using the trial wavefunction as

$$E[H] = \langle H \rangle = \frac{\int \mathrm{d}\vec{R}\, \Psi_T^* H \Psi_T}{\int \Psi_T^* \Psi_T}. \tag{7}$$

The probability of $\vec{R}$, under the trial wavefunction, is

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

We finally define a new quantity, called the local energy:

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

We can now rewrite $\langle H \rangle$ as follows:

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

where R_i are randomly drawn positions from the PDF $P(\vec{R}, \vec{\alpha})$. We have therefore that estimating the average value of E_L yields an approximated value for $\langle H \rangle$, which must 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 Finding an Analytical Expression for E_L

The hard part of the expression for E_L is

$$\frac{1}{\Psi_L}\sum_k^N \nabla_k^2 \Psi_L. \tag{11}$$

To get going, we rewrite the wavefunction as

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

where $r_{ij} = \|\vec{r}_{ij}\| = \|\vec{r}_i - \vec{r}_j\|$, $u(r_{ij}) = \ln f(r_{ij})$, and $\phi(\vec{r}_i) = g(\alpha, \beta, \vec{r}_i)$. In order to evaluate this, we first evaluate some expressions we will need.

$$\begin{aligned}
\boldsymbol{\nabla}_k \Psi_T(\vec{r}) &= \boldsymbol{\nabla}_k \prod_i \phi(\vec{r}_i)\exp\left(\sum_{i<j} u(r_{ij})\right) \\
&= \prod_{i\neq k} \phi(\vec{r}_i)\exp\left(\sum_{i<j} u(r_{ij})\right)\boldsymbol{\nabla}_k\phi(\vec{r}_k) + \prod_i \phi(\vec{r}_i)\boldsymbol{\nabla}_k\exp\left(\sum_{i<j} u(r_{ij})\right) \\
&= \Psi_T\left[\frac{\boldsymbol{\nabla}_k\phi(\vec{r}_k)}{\phi(\vec{r}_k)} + \sum_{j\neq k}\boldsymbol{\nabla} u(r_{kj})\right]. \\
\boldsymbol{\nabla}_k u(r_{kj}) &= u'(r_{kj})\boldsymbol{\nabla}_k\sqrt{\|\vec{r}_k - \vec{r}_j\|^2} \\
&= u'(r_{kj})\frac{1}{2r_{kj}}\boldsymbol{\nabla}_k\left(\|\vec{r}_k\|^2 - 2\vec{r}_k\cdot\vec{r}_j + \|r_j\|^2\right) \\
&= u'(r_{kj})\frac{\vec{r}_{kj}}{r_{kj}}. \\
\boldsymbol{\nabla}_k\cdot\frac{\vec{r}_{kj}}{r_{kj}} &= \frac{\boldsymbol{\nabla}_k\cdot(\vec{r}_k - \vec{r}_j) - (\vec{r}_k - \vec{r}_j)\cdot\boldsymbol{\nabla}_k r_{kj}}{r_{kj}^2} \\
&= \frac{2}{r_{kj}}. \\
\nabla_k^2 u(r_{kj}) &= \boldsymbol{\nabla}_k\cdot u'(r_{kj})\frac{\vec{r}_{kj}}{r_{kj}} \\
&= u'(r_{kj})\frac{2}{r_{kj}} + \frac{\vec{r}_{kj}}{r_{kj}}\cdot\boldsymbol{\nabla}_k u'(r_{kj}) \\
&= u''(r_{kj}) + \frac{2}{r_{kj}}u'(r_{kj}).
\end{aligned}$$

$$
\begin{aligned}
u'(r_{ij}) &\equiv \frac{\partial}{\partial r_{ij}} \ln\left(1 - \frac{a}{r_{ij}}\right) \\
&= \frac{a}{r_{ij}(r_{ij} - a)}. \\
u''(r_{ij}) &= \frac{\partial^2}{\partial r_{ij}^2} \ln\left(1 - \frac{a}{r_{ij}}\right) \\
&= \frac{a(a - 2r_{ij})}{r_{ij}^2(r_{ij} - a)^2}. \\
\frac{\boldsymbol{\nabla}_k \phi(\vec{r}_k)}{\phi(\vec{r}_k)} &= -2\alpha \begin{pmatrix} x \\ y \\ \beta z \end{pmatrix}. \\
\frac{\nabla_k^2 \phi(\vec{r}_k)}{\phi(\vec{r}_k)} &= 2\alpha\big[2\alpha x^2 + 2\alpha y^2 + 2\alpha\beta^2 z^2 - d(\beta)\big].
\end{aligned}
$$

where, $d(\beta) = 1, 2$, or $2 + \beta$ for one, two and three dimensions, respectively. Then, with all this in place, we get:

$$
\begin{aligned}
\frac{1}{\Psi_L}\nabla_k^2 \Psi_L &= \frac{1}{\Psi_L}\boldsymbol{\nabla}_k \cdot \left\{\Psi_T\left[\frac{\boldsymbol{\nabla}_k \phi(\vec{r}_k)}{\phi(\vec{r}_k)} + \sum_{j\neq k} \boldsymbol{\nabla} u(r_{kj})\right]\right\} \\
&= \frac{\nabla_k^2 \phi(\vec{r}_k)}{\phi(\vec{r}_k)} + \frac{\boldsymbol{\nabla}_k(\phi(\vec{r}_k)) \cdot \left(\sum_{j\neq k} \boldsymbol{\nabla}_k u(r_{kj})\right)}{\phi(\vec{r}_k)} + \sum_{j\neq k} \nabla_k^2 u(r_{kj}) \\
&+ \left[\left(\frac{\boldsymbol{\nabla}_k \phi(\vec{r}_k)}{\phi(\vec{r}_k)} + \sum_{j\neq k} \boldsymbol{\nabla}_k u(r_{kj})\right) \cdot \left(\sum_{j\neq k} \boldsymbol{\nabla}_k u(r_{kj})\right)\right] \\
&= \frac{\nabla_k^2 \phi(\vec{r}_k)}{\phi(\vec{r}_k)} + 2\frac{\boldsymbol{\nabla}_k \phi(\vec{r}_k)}{\phi(\vec{r}_k)} \cdot \sum_{j\neq k}\left(\frac{\vec{r}_{kj}}{r_{kj}} u'(r_{kj})\right) \\
&+ \sum_{i,j\neq k} \frac{\vec{r}_{ki} \cdot \vec{r}_{kj}}{r_{ki} r_{kj}} u'(r_{ki}) u'(r_{kj}) + \sum_{j\neq k}\left(u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj})\right) \\
&= 2\alpha\big[2\alpha x^2 + 2\alpha y^2 + 2\alpha\beta^2 z^2 - \beta - 2\big] \\
&- 4\alpha \begin{pmatrix} x \\ y \\ \beta z \end{pmatrix} \cdot \left[\sum_{j\neq k} \frac{\vec{r}_{kj}}{r_{kj}} \frac{a}{r_{kj}(r_{kj} - a)}\right] \\
&+ \sum_{i,j\neq k} \frac{\vec{r}_{ki} \cdot \vec{r}_{kj}}{r_{ki} r_{kj}} \frac{a}{r_{ki}(r_{ki} - a)} \frac{a}{r_{kj}(r_{kj} - a)} \\
&+ \sum_{j\neq k}\left(\frac{a(a - 2r_{kj})}{r_{kj}^2(r_{kj} - a)^2} + \frac{2}{r_{kj}} \frac{a}{r_{kj}(r_{kj} - a)}\right).
\end{aligned}
\tag{13}
$$

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:

$$\begin{aligned} E_L &= \frac{1}{\Psi_T} H \Psi_T \\ &= \sum_i V_{ext}(\vec{r}_i) + \sum_{i<j} V_{int}(\vec{r}_i, \vec{r}_j) - \frac{\hbar^2}{2m} \sum_k \frac{1}{\Psi_T} \nabla_k^2 \Psi_T \end{aligned} \tag{14}$$

where we substitute in (13) in the final sum.