Variational Monte Carlo studies of quantum mechanical systems (WIP title)

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Abstract

1 Introduction

The ground state energy of different amounts of trapped, hard spheres Bose gas atoms are evaluated using Variational Monte Carlo (VMC) numerical calculations. The use of this, and other, numerical methods have been and will continue to be important in order to be able to preform such experiments/simulations, witch would not be possible otherwise(??)

2 Theory

2.1 The system in question

The system in question is a hard sphere Bose gas located in a potential well. The potential is an *elliptical harmonic trap*, described for each particle by

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m\left(\omega_{\text{ho}}^2(r_x^2 + r_y^2) + \omega_z^2 r_z^2\right). \tag{1}$$

Here, $\mathbf{r}$ is the position of the particle. Note that setting $\omega_{\text{ho}} = \omega_z$ results in eq. (1) evaluating to $V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m\omega_{\text{ho}}^2 r^2$, which represents the *spherical* case of the elliptical harmonic trap. As a simplification, we hereby denote the spherical case as (S) and the general elliptical case as (E).

In addition to this external potential, we represent the inter-boson interactions with the following pairwise, repulsive potential:

1

$$V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases}. \tag{2}$$

Eq. (1) and eq. (2) evaluate to the following two-body Hamiltonian:

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

The index notation used here is described in A.2.1. The term $-\frac{\hbar^2}{2m}\nabla_i^2$ is the operator stemming from the kinetic energy of the system.

2.1.1 The variational principle

Here is some more text.

Given this Hamiltonian, we can introduce the concept of a *trial wave function* $\Psi_T(\alpha)$. This is a normalized ansatz to the ground state wave function parametrized by the parameter(s) α. This gives us a way of deploying the *variational principle* by varying said parameter α to our needs:

We know that for any normalized function Ψ_T, the expected energy is higher than the ground state energy (as proved in [1] on p. 293-294), viz.

$$\langle E(\alpha) \rangle = \langle \Psi_T(\alpha)|H|\Psi_T(\alpha) \rangle \geq E_0 = \langle \Psi_0|H|\Psi_0 \rangle. \tag{3}$$

Thus, minimizing over α will give an approximation of the true ground state (perhaps even an accurate answer).

2.1.2 Wave function of the system

For the abovementioned system, containing N particles, we use the following trial wave function:

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

where

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

and

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

Once again, note the index notation explained in A.2.1.

2.2 Importance sampling

Importance sampling, compared to the brute force Metropolis sampling, sets a bias on the sampling, leading it on a better path. This means that the desired standard deviation is acquired after fewer Monte Carlo cycles.

For our quantum mechanical scenario with boson particles in a magnetic trap, the bias has its root in the so-called quantum force. This quantum force pushes the walker (the boson particle) to the regions where the trail wave function is large. It is clear that this yields a faster convergence, compared to the Metropolis algorithm where the walker has the same probability of moving in all directions.

The quantum force $\mathbf{F}$ is given by the formula

$$\mathbf{F} = 2\frac{1}{\Psi_T}\nabla\Psi_T,$$

which is derived from the Fokker-Planck equation, using the Langevin equation to generate the next step with Euler's method, and by making the probability density converge to a stationary state.

2.2.1 Fokker-Planck

For one particle (or walker), the one-dimensional Fokker-Planck equation for a diffusion process is:

$$\frac{\partial P}{\partial t} = D\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} - F\right)P(x,t)$$

Where $P(x,t)$ is is a time-dependent probability density, D is the diffusion coefficient and F is a drift term which is our case is driven by the quantum force.

2.2.2 Langevin equation

The Langevin equation solution gives the position of the walker in the next timestep. The Langevin equation is:

$$\frac{\partial x(t)}{\partial t} = DF(x(t)) + \eta$$

Converting this to a function yielding the new position y in a computational manner, we use Euler's method.

$$y = x + DF(x)\Delta t + \xi\sqrt{\Delta t}$$

Where the symbols represent: |Variable|Description| |—|—| |y | New position| |x | Current position | |DF(x) | Diffusion and Drift at the old possition| |D | In AU*: 1/2, from the kinetic energy operator| |Δt | Chosen time-step| |ξ | Gaussian random variable | * Atomic Units Examples of timesteps giving stable values of the ground state energy is $\Delta t \in [0.001, 0.01]$

2.2.3 Fokker-Planck and Langevin equation in importance sampling

In order to use these equations for our importance sampling, we start with the original Fokker-Planck equation.

After inserting D as the diffusion coefficient and $\mathbf{F_i}$ as component i of the drift velocity, we can make the probability density converge to a stationary state by setting its partial derivative over time to zero.

$$\frac{\partial P}{\partial t} = \sum_i D \frac{\partial}{\partial \mathbf{x_i}} \left(\frac{\partial}{\partial \mathbf{x_i}} - \mathbf{F_i} \right) P(\mathbf{x}, t)$$

Where then $\frac{\partial P}{\partial t} = 0$, and by expanding the parenthesis and moving the double partial derivative over to the other side, we obtain:

$$\frac{\partial^2 P}{\partial \mathbf{x_i}^2} = P \frac{\partial}{\partial \mathbf{x_i}} \mathbf{F_i} + \mathbf{F_i} \frac{\partial}{\partial \mathbf{x_i}} P$$

By inserting $g(\mathbf{x})\frac{\partial P}{\partial x}$ for the drift term, $\mathbf{F}$, we get

$$\frac{\partial^2 P}{\partial \mathbf{x_i}^2} = P \frac{\partial g}{\partial P} \left(\frac{\partial P}{\partial \mathbf{x}_i} \right)^2 + Pg \frac{\partial^2 P}{\partial \mathbf{x}_i^2} + g \left(\frac{\partial P}{\partial \mathbf{x}_i} \right)^2$$

Where again the left hand side can be set to zero to comply with the fact that at a stationary state, the probability density is the same for all walkers. [THIS MUST BE FALSE??? WHY can we really set this term to zero??]

For this to be solvable, the remaning terms have to cancel each other. This is only possible when $g = P^{-1}$, which gives the aforementioned quantum force, $\mathbf{F}$,

$$\mathbf{F} = 2 \frac{1}{\Psi_T} \nabla \Psi_T.$$

From here, The Green's function is employed as

$$G(y, x, \Delta t) = \frac{1}{(4\pi D \Delta t)^{3N/2}} \exp \left(-(y - x - D\Delta t F(x))^2 / 4D\Delta t \right)$$

Which will be part of the [insert name..], $q(y, x)$ as

$$q(y, x) = \frac{G(x, y, \Delta t) \left| \Psi_T(y) \right|^2}{G(y, x, \Delta t) \left| \Psi_T(x) \right|^2}$$

2.3 Analytical

2.3.1 Local energy simple Gaussian wave function

As a test case to be compared against our numerical implementation, we want to find an analytical expression for the energy of the trial wave function(Ref)(local

energy). We only study the harmonic oscillator potential and disregard the two-body potential. This is simply done by setting the parameter $a = 0$ which by (2) gives $V_{\text{int}} = 0$. First β is set to 1 to find the relevant local energies for one to three dimensions for both one and N particles. The simplest Gaussian wavefunction then becomes:

$$\Psi_T(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_N}, \, , \,) = \prod_i \exp(-\alpha r_i^2).$$

The energy is here given by

$$E_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})} H \Psi_T(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})} \left[\sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i) \right) \right] \Psi_T(\mathbf{r})$$

$$= \frac{1}{\Psi_T(\mathbf{r})} \left[\sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 \Psi_T(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}_i) \Psi_T(\mathbf{r}) \right) \right].$$

We simplify $\nabla_i^2 \Psi_T$ as shown in A.3.1 to get

$$\nabla^2 \Psi_t(\mathbf{r}) = -2\alpha \Psi_T \left(\dim - 2\alpha \mathbf{r}_i^2 \right), \tag{5}$$

where dim is the dimension of the system (1, 2 or 3). Given eq. (5), we find that the local energy for N particles in the case of the simple Gaussian wavefunction is

$$E_L(\mathbf{r}) = \frac{\hbar^2}{m} \alpha N \dim + \left(\frac{1}{2} m \omega_{\text{ho}}^2 - 2\alpha^2 \right) \sum_i^N \mathbf{r}_i^2, \tag{6}$$

as shown in A.3.2. We can simplify this even further by scaling, namely setting $\hbar = m = 1$, which gives us the equation

$$E_L(\mathbf{r}) = N\alpha \dim + \left(\frac{1}{2} m \omega_{\text{ho}}^2 - 2\alpha^2 \right) \sum_i^N \mathbf{r}_i^2 \tag{7}$$

An even simpler analytic expression is obtained by setting $\omega_{\text{ho}} = 1$ and taking the derivate of the local energy with respect to r_i, giving $\alpha = 0.5$.

$$E_L = \frac{N \dim}{2}$$

2.3.2 Drift force

The following expression for the drift force will be used to **explanation**

$$F = \frac{2\nabla_k \Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = -4\alpha \mathbf{r}_k$$

applying the gradient operator to the trail wavefunction is already shown (appendix: Second derivative of trial wave function).

##Local energy for full wavefunction With $\beta \neq 0$ and a > 0 the wave function becomes a bit more complicated as the potential/Gaussian can be can now be elliptical and the wave function contains the Jastrow factor. Difficult to find an analytical expression for the derivate of the trail wave function.

$$E_L(\mathbf{r}) \frac{1}{\Psi_T(\mathbf{r})} \sum_i^N \nabla_i^2 \Psi_T(\mathbf{r}),$$

Rewriting the full wave function

$$\Psi_T(\mathbf{r}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N, \alpha, \beta) = \left[\prod_i g(\alpha, \beta, \mathbf{r}_i) \right] \left[\prod_{j<k} f(a, |\mathbf{r}_j - \mathbf{r}_k|) \right],$$

to the following

$$\Psi_T(\mathbf{r}) = \left[\prod_i^N \phi(\mathbf{r}_i) \right] \exp\left(\sum_{i<j} u(r_{ij}) \right)$$

where

$$r_{ij} = |r_i - r_j|$$
$$u(r_{ij}) = \ln f(r_{ij})$$
$$\phi(\mathbf{r}_i) = \exp[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)] = g(\alpha, \beta, \mathbf{r}_i)$$

The first derivative for the k'th particle then is a bit tricky to calculate, so the result will be presented her while the full calculation is in **REF APPENDIX**. The analytical expression becomes

$$\nabla_k \Psi_T(\mathbf{r}) = \nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k}^N \phi(\mathbf{r}_k) \right] \exp\left(\sum_{j<m}^N u(r_{jm}) \right) + \left[\prod_i^N \phi(\mathbf{r}_i) \right] \exp\left(\sum_{j<m}^N u(r_{jm}) \right) \sum_{l \neq k}^N \nabla_k(r_{kl}),$$

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The second derivative:

The Laplacian is obtained

3 Method

3.1 Variational Monte Carlo

4 Results

5 Discussion

6 Conclusion

A Appendix

A.1 Source code

All source code for both the Rust VMC implementation and this document is found on the following GitHub Repository

https://github.com/kmaasrud/vmc-fys4411

A.2 Notation and other explanations

A.2.1 Index notation for sums and products

For products and sums, the following convention is used:

$$\sum_{i<j}^{N} = \sum_{i=1}^{N} \sum_{j=i+1}^{N}, \quad \text{or} \quad \prod_{i<j}^{N} = \prod_{i=1}^{N} \prod_{j=i+1}^{N}$$

A.3 Intermediate calculations

A.3.1 Second derivative of trial wave function

$$
\begin{aligned}
\nabla_i^2 \Psi_T(\mathbf{r}) &= \nabla_i \cdot \left[\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i} \right] \Psi_T(\mathbf{r}) \\
&= \nabla_i \cdot \left[\frac{\partial}{\partial x_i} \exp\left(-\alpha \mathbf{r}_i^2\right), \frac{\partial}{\partial y_i} \exp\left(-\alpha \mathbf{r}_i^2\right), \frac{\partial}{\partial z_i} \exp\left(-\alpha \mathbf{r}_i^2\right) \right] \\
&= \nabla_i \cdot \left[-2\alpha x_i \exp\left(-\alpha \mathbf{r}_i^2\right), -2\alpha y_i \exp\left(-\alpha \mathbf{r}_i^2\right), -2\alpha z_i \exp\left(-\alpha \mathbf{r}_i^2\right) \right] \\
&= -2\alpha \left[\exp\left(-\alpha \mathbf{r}_i^2\right)(1 - 2\alpha x_i^2), \exp\left(-\alpha \mathbf{r}_i^2\right)(1 - 2\alpha y_i^2), \exp\left(-\alpha \mathbf{r}_i^2\right)(1 - 2\alpha z_i^2) \right] \\
&= -2\alpha \Psi_T \left[(1 - 2\alpha x_i^2), (1 - 2\alpha y_i^2), (1 - 2\alpha z_i^2) \right] \\
&= -2\alpha \Psi_T \sum_{d=x,y,z} 1 - 2\alpha d_i^2 \\
&= -2\alpha \Psi_T (\dim -2\alpha \mathbf{r}_i^2)
\end{aligned}
$$

A.3.2 Local energy for Gaussian wave function

Starting with

$$
E_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})} \left[\sum_i^{N} \left(\frac{-\hbar^2}{2m} \nabla_i^2 \Psi_T(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}_i) \Psi_T(\mathbf{r}) \right) \right],
$$

and using the result from A.3.1, this results in:

$$E_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})} \left[\sum_i^N \left(\frac{\hbar^2 \alpha}{m} (\dim - 2\alpha \mathbf{r}_i^2) + \frac{1}{2} m \omega_{\text{ho}}^2 \mathbf{r}_i^2 \right) \Psi_T(\mathbf{r}) \right]$$

$$= \frac{\hbar^2}{m} \alpha N \dim + \left(\frac{1}{2} m \omega_{\text{ho}}^2 - 2\alpha^2 \right) \sum_i^N \mathbf{r}_i^2$$

References

[1]   David. J. Griffiths, *Introduction to Quantum Mechanics*. 2005.

[2]   K. M. Aasrud, A. S. Rongve, and A. M. Raniseth, "Project 3." Oct. 2019, [Online]. Available: https://github.com/kmaasrud/gq-mcm-fys3150/blob/master/doc/Project-3_Aasrud-Raniseth-Rongve.pdf.