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

Anna Stray Rongve        Knut Magnus Aasrud
Amund Midtgard Raniseth

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**Abstract**

# 1 Introduction

# 2 Theory

## 2.1 The system described

The system in question is a hard sphere Bose gas. The system is affected by an external potential - an *elliptical harmonic trap* - that is described for each particle by the following equation:

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

$\mathbf{r}$ describes 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. In addition to this external potential, we represent the inter-boson interactions with the following pairwise, repulsive potential:

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

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.

### 2.1.1 The variational principle

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) $\alpha$. This gives us a way of deploying the *variational principle* by varying said parameter $\alpha$ to our needs. We know that for any normalized function $\Psi_T$, the expected energy is higher than the ground state energy (proved in Griffiths 2005 on p. 293-294). So

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

Thus minimizing over $\alpha$ 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.

## 2.3 Analytical

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 $\beta$ 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:

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

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 the Gaussian wavefunction is

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

as shown in A.3.2. We can simplify this even further by scaling, namely setting $\hbar = m = \omega_{\text{ho}}^2 = 1$, which gives us the equation

$$E_L(\mathbf{r}) = (\alpha \cdot \dim -3\alpha^2) \sum_i^N \mathbf{r}_i^2 \tag{7}$$

### 2.3.1 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 in eq (REF).

# 3 Method

## 3.1 Importance sampling

With importance sampling, the walk in the coordinate space will be biased by the trail wave function.(hvis jeg bare forsto hva jeg skreiv nå..) We will base our approach on the Fokker-Planck and Langevin equations, which is used for trajectory generation in the coordinate space. (Er dette for mye kopiert fra Importance Sampling?)

For one particle (sometimes also called 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.

From here, the Langevin equation is solved using Euler's method, which will give us the new positions in coordinate space.

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

Where $\eta$ is a random variable. This gives the new position:

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

Where the letters and symbols mean: |Variable|Description| |—|—| |y | new position| |x |old position |DF(x) | Diffusion and Drift at the old possition| |$\Delta$t | Chosen time-step| |$\xi$ | Gaussian random variable | Examples of timesteps giving stable values of the ground state energy is $\Delta t \in [0.001, 0.01]$

# 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:

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

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

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

## B   Syntax

I'm sure you're both familiar with the common Markdown syntax, and this applies just as well here. Pandoc exports links to the compiled PDF, so I often use them liberally, like this. If you want *inline math*, you just write a set of dollar signs, like this: $f(x) = \sin(x)$. Most commonly though, you'll probably want *display math*, which is just as simple to write. Be sure to have a couple of newlines as padding, and just use a double set of dollar signs, like this:

$$E(\alpha) = \frac{\langle \psi(\alpha) | \mathcal{H} | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle}$$

By default, these are not numerated (which I think is sensible). However, if you want them numerated, you just use the following syntax to assign a label

$$E_L(X) = \frac{\mathcal{H} \psi(X, \alpha)}{\psi(X, \alpha)}, \tag{8}$$

and then reference the equation by using the same label. See eq. (8) (beware that this will not show up in the Markdown Preview pane. You'll need to compile the document to see the result).

One thing I find quite useful is to use footnotes throughout the document to give short insights (especially in the theory part). This is simple with Pandoc; just use this syntax[1]. In addition, we can site all references (defined in the `kodb.yaml`-file) with this syntax (see Aasrud, Rongve, and Raniseth 2019).

## References

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

Griffiths, David. J. 2005. *Introduction to Quantum Mechanics.*

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[1] Welcome to the footer! How are you?