Project 1 - Monte Carlo

Authors goes here

I. INTRODUCTION

The GitHub repository is available here: https://github.com/Caronthir/FYSSTK4155/projects/.

II. THEORY

A. Variational Monte Carlo

In order to find a good candidate wavefunction for a given potential, one can employ the *variational principle*. One starts by guessing a trial wavefunction $|\Psi_T\rangle$ and estimating the trial energy, which is guaranteed to be equal to or higher than the true ground state energy E_0:

$$E_0 \leq E = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \tag{II.1}$$

If $|\Psi_T\rangle$ is an eigenfunction of the Hamiltonian, the variance σ^2 will be minimal

$$\sigma^2 = \frac{\langle \Psi_T | H^2 | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} - \left(\frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \right)^2 = 0$$

The variational principle expands on this idea by letting $|\Psi_T\rangle$ be a functional class of a *variational parameter* α. By varying α one can find the optimal trial wavefunction within the functional class by minimizing σ^2.
Only a small collection of potentials have analytical solution using the variational principle. For most potentials, one must numerically integrate (II.1) using Monte Carlo integration.
For a stochastic variable x with probability density function $p(x)$, the average $\langle x \rangle$ is defined as

$$\langle x \rangle = \int_{\mathbb{R}} x p(x) \mathrm{d}x$$

By sampling the stochastic variable M times, the average can be approximated by

$$\langle x \rangle = \int_{\mathbb{R}} x p(x) \mathrm{d}x \approx \frac{1}{M} \sum_{i=1}^{M} x_i p(x_i)$$

Applying this to an observable $\mathcal{O}$, we have

$$\begin{aligned} \langle \mathcal{O} \rangle &= \langle \Psi | \mathcal{O} | \Psi \rangle \\ &= \int \mathrm{d}\mathbf{r} \Psi^* \mathcal{O} \Psi \\ &= \int \mathrm{d}\mathbf{r} |\Psi|^2 \frac{1}{\Psi} \mathcal{O} \Psi \\ &= \frac{1}{M} \sum_{i=1}^{M} p(\mathbf{r}) \mathcal{O}_L \end{aligned}$$

where $|\Psi|^2$ is defined as the probability density function, and $\frac{1}{\Psi}\mathcal{O}\Psi$ the *local operator*.
The local trial energy can then be defined as

$$E_L = \frac{1}{\Psi_T} H \Psi_T$$

which can be computed using Monte Carlo integration as

$$\langle E_L \rangle \approx \frac{1}{M} \sum_{i=1}^{M} p(\mathbf{r}_i) E_L(\mathbf{r}_i)$$

The goal is therefore to minimize minimizing $\sigma^2 = \langle E_L^2 \rangle - \langle E_L \rangle^2$ over the variational parameter α.

B. Gradient Descent

The optimal value for the variational parameter is found by gradient descent.

C. The System

1. The Potentials

The Hamiltonian under investigation describes N bosons in a potential trap, and is on the form

$$H = \sum_{i=1}^{N} \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i) \right) + \sum_{i<j}^{N} V_{\text{int}}(\mathbf{r}_i, \mathbf{r}_j)$$

where V_{ext} is the external potential of the trap while V_{int} is the internal potential between the particles. The external potential has an elliptical form, being anisotropic in the z-direction:

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2} m \left(\omega \left[x^2 + y^2 \right] + \omega_z z^2 \right) \tag{II.2}$$

The internal potential is a hard shell potential, being infinite for distances where two bosons overlap:

$$V_{\text{int}} = \begin{cases} \infty, & \text{for } |r_i - r_j| \leq 0 \\ 0, & \text{otherwise} \end{cases}$$

2. The Trial Wavefunction

The elliptical spherical trap (II.2) represents a harmonic oscillator. As the trial wavefunction should be as close as possible to the expected true wavefunction, a reasonable guess at its shape is then the eigenfunction of harmonic oscillators, namely Gaussian functions. For a N-bosonic system the trial wavefunction is therefore

$$\begin{aligned} h(\mathbf{r}_1, \ldots, \mathbf{r}_N, \alpha, \beta) &= \prod_{i=1}^{N} g(\mathbf{r}_i, \alpha, \beta) \\ &= \exp\left\{ -\sum_{i=1}^{N} \left(x_i^2 + y_i^2 + \beta z_i^2 \right) \right\} \end{aligned}$$

with g the onebody function. The internal potential should cause the wavefunction to decrease continuously down to zero as the distance of two particles goes to zero. Once such possible function is

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

Combining both potential contributions, the complete trial wave function is therefore

$$\Psi_T(\mathbf{r}, \alpha, \beta, a) = \exp\left\{ -\alpha \sum_{i=1}^{N} \left(x_i^2 + y_i^2 + \beta z_i^2 \right) \right\} \prod_{i<j}^{N} f(a, \mathbf{r}_i, \mathbf{r}_j)$$

3. Analytical Solutions

D. Drift Force

E. Onebody Density

III. METHOD

A. Outline of Program

B. Non Interacting Potentials

C. Interacting Potentials

D. Statistical Treatment

IV. RESULTS

A. Non Interacting Potentials

B. Interacting Potentials

C. Local Energy

D. Optimal Parameter α

E. Onebody Density

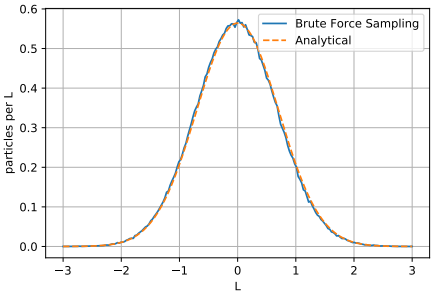
V. RESULTS AND DISCUSSION

A. Sampling of States using Metropolis

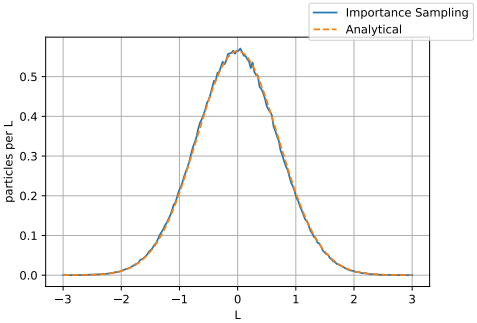
In Figure V.1 we see that both brute force sampling and importance sampling manage to approximate the onebody density derived from the non-interacting trial wave function: Aside from the statistical noise introduced by the finite number of Monte-Carlo cycles, the approximated densities follow the analytical result closely. Figure Figure V.2 demonstrates that this also scales to more particles and dimensions, as seen from the radial onebody density of two particles in three dimensions.

B. Blocking of Local Energy

In Figure V.3, we see the effect of applying blocking on the local energy data before calculating the variance of the estimator (kilde). Although the local energies are sampled from an approximately correct distribution, as indicated by Figure V.2, the data is produced by moving a single electron at a time. Moreover, the move may even be rejected by the metropolis algorithm. Thus, the data is highly correlated, causing an underestimation of the variance as seen for the

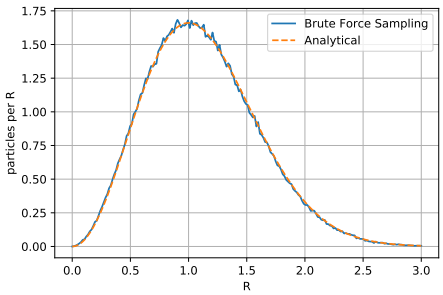


Approximation of onebody density using Metropolis brute force sampling vs analytical(kilde)

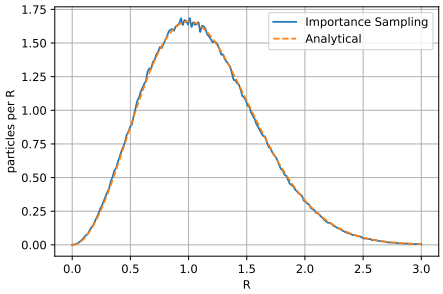


Approximation of onebody density using Metropolis importance sampling vs analytical

Figure V.1: One-body density of 1 boson in 1 dimmension, using $N = 1e6$ cycles, $\omega = 1$, $\alpha = 0.5$.

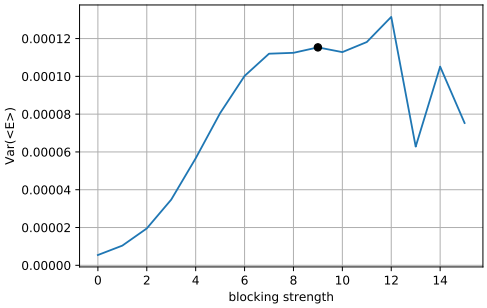


Approximation of radial onebody density using Metropolis brute force sampling vs analytical

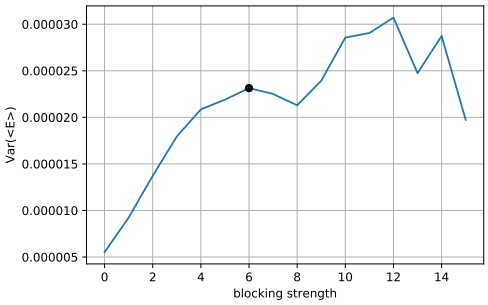


Approximation of radial onebody density using Metropolis importance sampling vs analytical

Figure V.2: Radial one-body density of 2 non-interacting bosons in 3 dimmensions, using $N = 1e6$ cycles, $\omega = 1$, $\alpha = 0.5$.



Brute Force Sampling



Importance Sampling

Figure V.3: Variance of the estimate of $< E >$ using blocked values of local energy at various strengths. The data has been produced for 2 non-interacting bosons i 3 dimension, using $N = 2^{17}$ cycles, $\alpha = 0.8$, $\omega = 1$, with and without importance sampling

unblocked data(blocking strength 0). After repeated blocking, the variance stabilizes when the data is approximately uncorrelated. Note that this happens at different strengths of blocking with and without importance sampling. This indicates that importance sampling creates data that are less correlated that

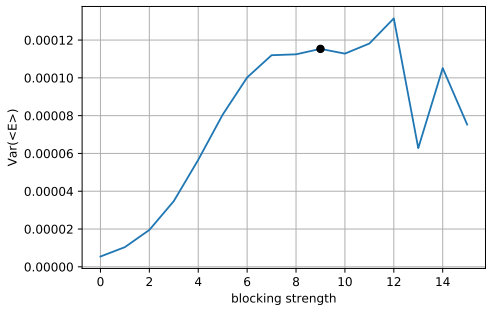


Figure V.4: Variance of the estimate of $< E >$ using blocked values of local energy at various strengths. The data has been produced for 2 non-interacting bosons i 3 dimension, using $N = 2^{17}$ cycles, $\alpha = 0.8$, $\omega = 1$, with and without importance sampling