# FYS9411 – Project 1

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# 1 Introduction

# 2 Background

## 2.1 Particle in harmonic trap

### 2.1.1 One particle

### 2.1.2 Many particles

### 2.1.3 Elliptic trap

## 2.2 Variational Monte Carlo

## 2.3 Importance sampling

## 2.4 Steepest decent algorithm

# 3 Analytic expressions

## 3.1 Local energy, no interaction

1, 2 and 3 dimensions for 1 and $N$ particles.

### 3.1.1 One dimension

The local energy, $E_L$, and the Hamiltonian, $H$, is given by the general expression

$$E_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})} H\Psi_T(\mathbf{r}), \quad H = \sum_i^N \frac{-\hbar^2}{2m}\nabla_i^2 + \tfrac{1}{2}m\omega_{ho}^2 r_i^2$$

For one particle $\mathbf{r}$ becomes

$$\mathbf{r} = x$$

where $x$ is the coordinate of the particle. The wave function and Hamiltonian becomes

$$\Psi_T(\mathbf{r}) = \Psi_T(x) = e^{-\alpha x^2}$$

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \tfrac{1}{2}m\omega_{ho}^2 x^2$$

which gives the local energy

$$E_L(x) = \frac{1}{\Psi_T(x)} H\Psi_T(x) = \frac{1}{e^{-\alpha x^2}}\Big(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \tfrac{1}{2}m\omega_{ho}^2 x^2\Big)e^{-\alpha x^2} = \frac{\hbar^2}{m}\alpha x + \tfrac{1}{2}m\omega_{ho}^2 x^2$$

For $N$ particles $\mathbf{r}$ becomes

$$\mathbf{r} = (x_1, x_2, ..., x_N)$$

### 3.2 Drift force

1, 2 and 3 dimensions.

### 3.3 Local energy, with interaction

3 dimensions for $N$ particles.

## 4 Calculating the ground state energy

### 4.1 Variational Monte Carlo

Variational Monte Carlo: starts with trial wave function, varies the parameters of the wave function to find an energy minimum

1, 2 and 3 dimensions, $N$=1, 10, 100, 500 (12 plot)

### 4.2 Importance sampling

1, 2 and 3 dimensions. Study the result as a function of the time step, $\delta t$ Discuss differences between brute force (Metropolis) and importance sampling.

### 4.3 Steepest decent algorithm

Finding optimal $\alpha$ before the Monte Carlo cycles. Compare the computation time.

### 4.4 Error analysis

### 4.5 Parallelizing the code

Compare computation time.

### 4.6 Repulsive interaction

Elliptic trap, introducing length and energy units. Show new expression for the Hamiltonian. What is the expression for $\gamma$? Vary $\alpha$ for $N$=10, 50, 100 and compare to ideal case. Compare results to Refs.

### 4.7 Onebody densities

Compute the onebody density with and without the Jastrow factor, and discuss the importance of the correlations induced by the Jastrow factor.

# 5 Conclusion

Summarize results.