Fys4110: Project 2

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Sammendrag

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1 Introduction

In this project I continue the study of many interacting particles in an isotropic two dimensional harmonic oscillator. In project 1 [1] I used Hartree-Fock methods to construct the Slater determinant of linear combinations of single particle non-interacting states that minimized the energy. In this project I would like to improve this estimate of the ground state by adding a Jastrow factor. Then the energy cannot be found with Hartree-Fock methods, but rather from direct integration of the Hamiltonean. I will do this using the Metropolis algorithm to pick out integration points. I will add a Jastrow factor with a free parameter, minimize the energy with respect to this parameter, and then calculate the energy of this new approximation of the ground state. In addition I will study the 2 particle case with a singly parametrized symmetric wavefunction instead of the Slater determinant.

2 Physical Problem

The full Hamiltonean of the problem with N particles and using atomic units is

$$H = \sum_i^N -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 + \sum_{i<j}^N \frac{1}{r_{ij}}, \tag{1}$$

where $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$.

2.1 2 Particle Case

For the two particle case I will aproximate the ground state with the parametrized trial wavefunction

$$\psi_T = A \exp\left(-\alpha\omega(r_1^2 + r_2^2) - \frac{r_{12}}{1 + \beta r_{12}}\right), \tag{2}$$

with α and β as free parameters.

2.2 Slater case

For the many particle case we will use the non-interacting ground state Slater determinant multiplied with a Jastrow factor with one free parameter. We could used Slater determinants from linear combinations of different non-interacting single particle states as found in [1] by Hartree-Fock methods, however this turned out to be to complicated. Instead we will compare the Hartree-Fock approach to adding a Jastrow factor to the ground state.

$$\psi_T = A \mathrm{Det}\left(\psi_1 \ldots \psi_N; \boldsymbol{r}_1 \ldots \boldsymbol{r}_N\right) \prod_{i<j}^N \exp\left(-\frac{a_{ij} r_{ij}}{1 + \beta r_{ij}}\right), \tag{3}$$

where ψ_i is the non-interacting single particle state with the ith lowest energy, and a_{ij} is 1 when the particles have anti-paralell spins and 1/3 when paralell. Since we are talking about spin 1/2 electrons there are two spin configurations for each spatial configuration for the single particle states that go into the Slater determinant. However the hamiltonean 1 is independent of spin. Wen can exploit this to simplify the wavefunction we use. If we let the $N/2$ first particles be in one spin state and the next $N/2$ in the other we may use a product of Slater determinants with only the particles in the same spin state in each:

$$\psi_T = A \mathrm{Det}\left(\psi_{1\downarrow}\dots\psi_{N/2\downarrow};r_1\dots r_{N/2}\right)\mathrm{Det}\left(\psi_{1\uparrow}\dots\psi_{N/2\uparrow};r_{N/2+1}\dots r_N\right)\prod_{i<j}^N \exp\left(-\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right). \quad (4)$$

In the 2 particle case this reduces to equation 2 with $\alpha = 1$.

3 Variational Monte-Carlo

4 The Metropolis Algorithm

The Metropolis algorithm is an algorithm for computing expectation values for functions of many variables efficiently. It is based on semi-randomly walking through the integration space and finding the value of the function at each point. Let $F(x_1,\dots,x_N)$ be the function we wish to find the expectation value of. Then

$$\langle F \rangle = \frac{\int F(x_1,\dots,x_N)p(x_1,\dots,x_N)\prod_{k=1}^N \mathrm{d}x_k}{\int p(x_1,\dots,x_N)\prod_{k=1}^N \mathrm{d}x_k}, \quad (5)$$

where $p(x_1,\dots,x_N)$ is the (generally) non-normalized probability density function. In our case p is $|\psi|^2$. One advantage with this method is that it does not require explicit normalization of the probability density.

4.1 Detailed Balance

The Metropolis algorithm may be derived by demanding that the Markov chain exhibits detailed balance. The criterion for detailed balance is

$$P(a)P(b|a) = P(b)P(a|b), \quad (6)$$

or rewritten

$$\frac{P(a)}{P(b)} = \frac{P(a|b)}{P(b|a)}. \quad (7)$$

We may split $P(a|b) = G(a|b)A(a|b)$, where $G(a|b)$ is the probability of proposing a move from b to a, while $A(a|b)$ is the probability of accepting a proposed move from b to a. The the detailed balance requirement may be rewritten as

$$\frac{A(a|b)}{A(b|a)} = \frac{P(a)G(b|a)}{P(b)G(a|b)}. \quad (8)$$

Now we choose an acceptance ratio that satisfies this requirement. The Metropolis choice is to use

$$A(a|b) = \min\left(1, \frac{P(a)G(b|a)}{P(b)G(a|b)}\right). \quad (9)$$

So the Metropolis algorithm for drawing points from a probability distrobution is

1. Draw a proposed move from the proposal distribution.

2. Evaluate the acceptance ratio a from equation 9.

3. Draw a random number $0 \le r < 1$ from a uniform distribution.

4. If $a > r$ accept the move. Else reject the move.

5. Save position

6. return to point 1.

4.2 Symmetric Proposal Density

If the proposal probality $G(a|b) = G(b|a)$ the proposal distribution is called symmetric and drops out of the acceptance ratio. Thus there is less to calculate for each loop in the algortihm. However symmetric proposal densities lead to many proposed steps being rejected, and thus to higher corelations between the points.

4.3 Importance Sampling

If we instead choose a non-symmetric proposal distribution we may choose one to maximise the acceptancerate. If we choose a proposaldistribution so that the probability of proposing a move into an area with a higher probability is higher than the probability of proposing a move into an area with a lower probability. In other words if $P(a) > P(b)$ then $G(a|b) > G(b|a)$.

4.4 Local Energy

In quantum mechanics the probability distribution is given by $|\psi|^2$ and the expectation value for an operator O is given by

$$\langle O \rangle = \frac{\int \psi^* O \psi \prod_i dx_i}{\int |\psi|^2 \prod_i dx_i}, \tag{10}$$

This is not exactly on the form of equation 5, but it can be rewritten in terms of local variables given by

$$O_L = \frac{1}{\psi} O \psi, \tag{11}$$

so that the expectation value is

$$\langle O \rangle = \frac{\int |\psi|^2 O_L \prod_i dx_i}{\int |\psi|^2 \prod_i dx_i}. \tag{12}$$

So the expectation value of the energy is given by

$$\langle E \rangle = \frac{\int |\psi|^2 E_L \prod_i dx_i}{\int |\psi|^2 \prod_i dx_i}, \tag{13}$$

with

$$E_L = \frac{1}{\psi} H \psi, . \tag{14}$$

4.5 2 Particle Case

In the two particle case with hamiltonean given by equation 1 and trial wavefunction by equation 2 the local energy is given by

$$E_L(\mathbf{r_1}, \mathbf{r_2}) = \left[\frac{1}{2}(1-\alpha)\omega(r_1^2 + r_2^2) + 2\alpha\omega \right] - \frac{a}{(1+\beta r_{12})^2} \left[\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1+\beta r_{12})} - \alpha\omega r_{12} \right] + \frac{1}{r_{12}}, \tag{15}$$

as shown in appendix A.2.

4.6 Slater Case

In the N particle case with hamiltonean given by equation 1 and trial wavefunction by equation 4 the local energy is given by

5 Implementation

5.1 Structure

5.2 Paralellization

6 Cost

7 Accuracy

7.1 Blocking

8 Benchmarks

8.1 2 Particle Case

A first test of the code is to check that when the interaction and jastrow factor are turned off and $\alpha = 1$ the energy is 2 with variance 0.

9 Results

10 Discussion

11 Conclusion

A Derivatives of the 2 particle trial wavefunction

In the course of the project we needed analytical expressions for different derivatives of the 2 particle trial wavefunction 2. I have collected the differentiations here.

A.1 Gradient

In order to compute the driftforce for importance sampling we needed

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial z},$$

where $z_i = x_1, x_2, y_1, y_2$. As ψ_T is an exponential

$$
\begin{aligned}
\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial z_i} &= \frac{\partial}{\partial z_i} \left(-\frac{1}{2}\alpha\omega(r_1^2 + r_2^2) + \frac{ar_{12}}{1 + \beta r_{12}} \right) \\
&= -\alpha\omega z_i + a \left(\frac{1}{1 + \beta r_{12}} - \frac{r_{12}\beta}{(1 + \beta r_{12})^2} \right) \frac{\partial r_{12}}{\partial z_i} \\
&= -\alpha\omega z_i + \frac{a}{(1 + \beta r_{12})^2} \frac{\partial r_{12}}{\partial z_i} \\
&= -\alpha\omega z_i + \frac{a}{(1 + \beta r_{12})^2} \frac{(z_i - z_j)}{r_{12}},
\end{aligned}
$$

where z_j is the coordinate of the other particle along the same dimension as z_i, so for example when $z_i = x_2, z_j = x_1$.

A.2 Laplacian

The local energy is defined as

$$E_L(\mathbf{r_1}, \mathbf{r_2}) = \frac{1}{\psi_T} H \psi_T.$$

In our case the Hamiltonean is

$$H = \sum_{i=1}^{2} -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 + \frac{1}{r_{12}}.$$

The laplacian is

$$\sum_i \nabla^2 = \sum_i \frac{\partial^2}{\partial z_i^2},$$

where z_i is the same as above.

Again since ψ_T is an exponential we have

$$\frac{1}{\psi_T}\frac{\partial^2 \psi_T}{\partial z_i^2} = \frac{\partial^2}{\partial z_i^2}\left(-\alpha\omega(r_1^2 + r_2^2)/2 + \frac{ar_{12}}{1+\beta r_{12}}\right) + \left(\frac{\partial}{\partial z_i}\left(-\alpha\omega(r_1^2 + r_2^2)/2 + \frac{ar_{12}}{1+\beta r_{12}}\right)\right)^2$$

$$= \frac{\partial}{\partial z_i}\left(-\alpha\omega z_i + \frac{a}{(1+\beta r_{12})^2}\frac{(z_i - z_j)}{r_{12}}\right) + \left(-\alpha\omega z_i + \frac{a}{(1+\beta r_{12})^2}\frac{(z_i - z_j)}{r_{12}}\right)^2$$

$$= -\alpha\omega + \frac{a}{(1+\beta r_{12})^2 r_{12}} - \frac{2a\beta(z_i - z_j)^2}{(1+\beta r_{12})^3 r_{12}^2} - \frac{a(z_i - z_j)^2}{(1+\beta r_{12})^2 r_{12}^3} + \alpha^2\omega^2 z_i^2 - \frac{2\alpha\omega a z_i(z_i - z_j)}{(1+\beta r_{12})^2 r_{12}} + \frac{a^2(z_i - z_j)^2}{(1+\beta r_{12})^4 r_{12}^2}.$$

So, because the ψ_T is symmetric under $1 \leftrightarrow 2$ and $x \leftrightarrow y$:

$$\frac{1}{\psi_T}\sum_i \nabla_i^2 \psi_T = \alpha\omega(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a^2}{(1+\beta r_{12})^4} + \frac{4a}{(1+\beta r_{12})^2 r_{12}} - \frac{4a\beta}{(1+\beta r_{12})^3} - \frac{2a}{(1+\beta r_{12})^2 r_{12}} - \frac{2\alpha\omega a r_{12}}{(1+\beta r_{12})^2}$$

and finally:

$$\frac{1}{\psi_T}\sum_i \nabla_i^2 \psi_T = \alpha\omega(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a}{(1+\beta r_{12})^2}\left[\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1+\beta r_{12})} - \alpha\omega r_{12}\right]$$

Using this expression we have the local energy as

$$E_L(\mathbf{r_1}, \mathbf{r_2}) = \left[\frac{1}{2}(1-\alpha)\omega(r_1^2 + r_2^2) + 2\alpha\omega\right] - \frac{a}{(1+\beta r_{12})^2}\left[\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1+\beta r_{12})} - \alpha\omega r_{12}\right] + \frac{1}{r_{12}},$$

where the second term contains the terms from the Jastrow-factor and the cross term and the third is the interaction term.

A.3 Derivatives w.r.t α and β

In order to find the optimal parameters α and β we needed the derivatives of ψ_T with respect to these.

$$\frac{1}{\psi_T}\frac{\partial \psi_T}{\partial \alpha} = -\frac{1}{2}\omega(r_1^2 + r_2^2).$$

$$\frac{1}{\psi_T}\frac{\partial \psi_T}{\partial \beta} = -\frac{ar_{12}^2}{(1+\beta r_{12})^2}.$$

B Derivatives of the N particle trial wavefunction

In the course of the project we needed analytical expressions for different derivatives of the N particle trial wavefunction 4. I have collected the differentiations here.

B.1 Gradient

We note that for any coordinate z_i only one of the determinants depends on it. So

$$\frac{\partial \psi_T}{\partial z_i} = \frac{\partial \text{Det}}{\partial z_i} J + \text{Det} \frac{\partial J}{\partial z_i}. \tag{16}$$

From section A.1 it is clear that

$$\frac{\partial J}{\partial z_i} = \left(\sum_{j \neq i} \frac{a_{ij}}{(1 + \beta r_{ij})^2} \frac{(z_i - z_j)}{r_{ij}} \right), \tag{17}$$

while

$$\frac{\partial \text{Det}}{\partial z_i} = \sum_{\sigma \in S_{N/2}} (-1)^{|\sigma|} \frac{1}{\psi_{\sigma(i)}(\boldsymbol{r_i})} \frac{\partial \psi_{\sigma(i)}(\boldsymbol{r_i})}{\partial z_i} \psi_{\sigma(1)}(\boldsymbol{r_1}) \dots \psi_{\sigma(N/2)}(\boldsymbol{r_{N/2}}) \tag{18}$$

B.2 Laplacian

B.3 Derivatives w.r.t α and β

In order to find the optimal parameters α and β we needed the derivatives of ψ_T with respect to these.

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \alpha} = -\frac{1}{2} \omega (r_1^2 + r_2^2).$$

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \beta} = -\frac{ar_{12}^2}{(1 + \beta r_{12})^2}.$$

Referanser

[1] K. Helland "Fys4411: Project 1" available at `https://github.com/khhelland/Fys4411/blob/master/1/rapport.pdf`

[2] E. Anisimovas and A. Matulis, "Energy spectra of few-electron quantum dots.", J. Phys.,10:601 615, 1998.

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[4] M. Hjort-Jensen,*Computational Physics: Hartree-Fock methods and introduction to Many-body Theory* found at `http://compphysics.github.io/ComputationalPhysics2/doc/pub/basicMB/pdf/basicMB-print.pdf` on the 16/03/17

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