

Project 2

Vilde Mari Reinertsen

Abstract

This is the abstract.

Contents

1	Introduction	2
2	Theory and method	2
2.1	Two particle system	2
2.2	More particles	3
2.3	One-body density	4
2.4	Virial theorem	5
2.5	Trap frequency	5
3	Results and discussion	5
3.1	Two electrons in two dimensions	5
3.1.1	Brute force sampling	5
3.1.2	Including importance sampling	6
3.1.3	Including optimization	6
3.1.4	Including interaction	7
3.2	Extending to more particles	7
3.2.1	Six particles	7
3.2.2	Twelve particles	7
	Appendices	7
A	Iteration - derivatives with regards to parameters	7
B	Dealing with the Slater determinant efficiently	7
B.1	Slater determinant	7
B.2	The Metropolis ratio	8
B.3	Updating the inverse of the Slater determinant	9
C	Energies	9
D	Hermite polynomials and the wavefunction derivatives	10

1 Introduction

2 Theory and method

In this project we investigate a fermionic system of $N=2, 6$ and 12 electrons. It is a so-called closed shell-system. The Hamiltonian used to model this system is

$$\hat{H} = \sum_{i=1}^N \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right) + \sum_{i<j} \frac{1}{r_{ij}}, \quad (1)$$

where

$$\hat{H}_0 = \sum_{i=1}^N \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right)$$

is the single particle part and

$$\hat{H}_1 = \sum_{i<j} \frac{1}{r_{ij}}, \quad (2)$$

represent the interaction potential between particles. The Hamiltonian is written in atomic units, which implies that $\hbar = 1, m = 1$, the unit of length is $a_0 = \dots$ and the unit of energy is \dots . We also have $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$ and ω is the oscillator frequency. Later we will study the dependence of the system on the oscillator frequency.

2.1 Two particle system

The single particle wave function in two dimensions is

$$\phi_{n_x, n_y}(x, y) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp(-\omega(x^2 + y^2)/2). \quad (3)$$

where the functions $H_{n_x}(\sqrt{\omega}x)$ are Hermite polynomials, while A is a normalization constant. The relevant Hermite polynomials in this project are listed in Appendix D. ω is the trap frequency.

For the lowest-lying state, E_{00} (see Fig. 1), we have $n_x = n_y = 0$ and an energy $\epsilon_{n_x, n_y} = \omega(n_x + n_y + 1) = \omega$, the total energy of the lowest-lying state is hence 2ω because there is room for two electrons with opposite spins.

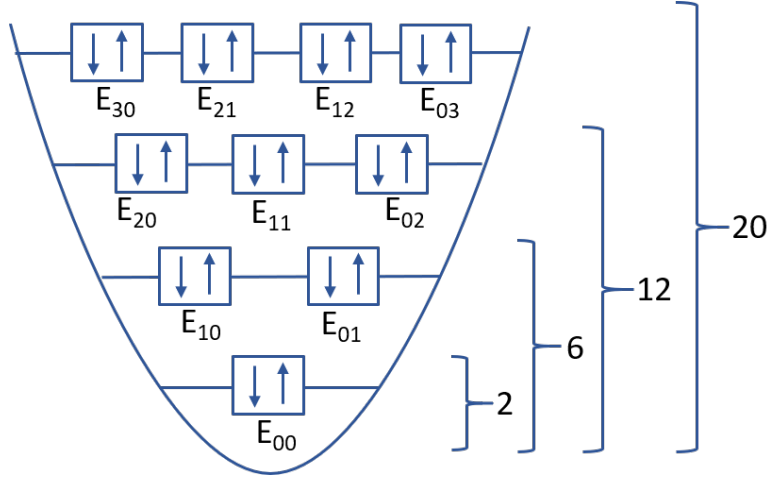


Figure 1: •

The expectation value can be found by solving the equation

$$\langle E \rangle = \frac{\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1, \mathbf{r}_2) \hat{H}(\mathbf{r}_1, \mathbf{r}_2) \psi_T(\mathbf{r}_1, \mathbf{r}_2)}{\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1, \mathbf{r}_2) \psi_T(\mathbf{r}_1, \mathbf{r}_2)}. \quad (4)$$

We will use Variational Monte Carlo (VMC) methods to evaluate the Eq. 4 [1]. The exact wave function for two not interacting electrons in the ground state is given by

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\omega(r_1^2 + r_2^2)/2),$$

where $r_i = \sqrt{x_i^2 + y_i^2}$ and C is a normalization constant. The trial wavefunction we use for the not interacting case is

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2).$$

with the parameter α . From the exact wave function we know that $\alpha = 1$ for the situation without interaction. On the other hand, for the interacting case, the trial wave function for the two-electron system is

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \exp\left(\frac{ar_{12}}{(1 + \beta r_{12})}\right), \quad (5)$$

where we introduce another parameter, β , and a spin factor, a . a is 1 when the two electrons have anti-parallel spins and $1/3$ when they have the parallel spins (this is not relevant before we introduce more particles to the system, as can be seen from Fig. 1).

2.2 More particles

Since we are looking at closed shell systems, the next amount of particles are six. We can see this from Fig. 1, there are room for two electrons with opposite spin in two different states, in addition to the two in the lowest lying state. The trial wave function is now given by

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_6) = \text{Det}(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_6(\mathbf{r}_6)) \prod_{i < j}^6 \exp\left(\frac{ar_{ij}}{(1 + \beta r_{ij})}\right), \quad (6)$$

where

$$\text{Det}(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_6(\mathbf{r}_6)) = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) & \cdots & \phi_6(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) & \cdots & \phi_6(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_6) & \phi_2(\mathbf{r}_6) & \cdots & \phi_6(\mathbf{r}_6) \end{vmatrix}$$

is the Slater determinant. This determinant occurs because electron are indistinguishable particles and they are antisymmetric The functions, $\phi_i(\mathbf{r}_j)$, are given by Eq. 3 and the notation is explained in Tab. 1.

Table 1: The relation between the notation used in the determinant (left) compared to Eq. 3 (right).

ϕ_1	$\phi_{n_x=0, n_y=0}$	ϕ_7	$\phi_{n_x=2, n_y=0}$
ϕ_2	$\phi_{n_x=0, n_y=0}$	ϕ_8	$\phi_{n_x=2, n_y=0}$
ϕ_3	$\phi_{n_x=1, n_y=0}$	ϕ_9	$\phi_{n_x=1, n_y=1}$
ϕ_4	$\phi_{n_x=1, n_y=0}$	ϕ_{10}	$\phi_{n_x=1, n_y=1}$
ϕ_5	$\phi_{n_x=0, n_y=1}$	ϕ_{11}	$\phi_{n_x=0, n_y=2}$
ϕ_6	$\phi_{n_x=0, n_y=1}$	ϕ_{12}	$\phi_{n_x=0, n_y=2}$

Similarly if we include another "shell" in our system we get 12 particles and the trial wavefunction is

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{12}) = \text{Det}(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_{12}(\mathbf{r}_{12})) \prod_{i < j}^{12} \exp\left(\frac{ar_{ij}}{(1 + \beta r_{ij})}\right). \quad (7)$$

The determinant have the same structure as for six particles and the relation to the single-particle wave functions are shown in Tab. 1.

2.3 One-body density

The radial one-body density is a measure of the spacial distribution of the electrons with respect to the distance from the middle of the harmonic oscillator trap. To calculate the radial one-body density, we want to sample the position of the electrons. The distance from the origin to a set cut-off is seperated into bins with a length Δr . For every Monte Carlo step, the distance between the electron's position and the origin is calculated, and the bin that corresponds to the current distance get a count. In the end, you have an array corresponding to the different bins with counts corresponding to how many times an electron was found to have that particular distance to the origin. This array is normalized by dividing by the number of Monte Carlo steps. However, to get the density, we have to divide the number in the bins with the area or volume the bin represents. Because we have two-dimensional

problem in this project and we calculate the radial one-body density, we divide bin i with the area $A = \pi(r_i + \Delta r)^2 - \pi r_i^2$ where r_i is distance from the origin to bin i . *normalized to the number of particles. Mention. Should happen automatically...*

2.4 Virial theorem

The virial theorem gives a relation between the time-average total kinetic energy, $\langle T \rangle$, and the time-average external potential energy, $\langle V_{ext} \rangle$, that is

$$2 \langle T \rangle = n \langle V_{ext} \rangle \quad (8)$$

where $V(r) = Br^n$. In our case when we do not include interaction $n = 2$ from the external potential term in Eq. 1, and therefore the average kinetic energy should be equal to the average potential energy. This can be used as a test to see if the simulations executed are correct.

2.5 Trap frequency

The trap frequency changes the external potential felt by the electrons. Figure 2 shows how a larger trap frequency, ω , results in a narrower external potential. In this narrow harmonic oscillator trap, the electrons are forced to be closer to each other. Later, we will investigate how ω affects the energy when the electrons are interacting with each other through the potential given in Eq. 2

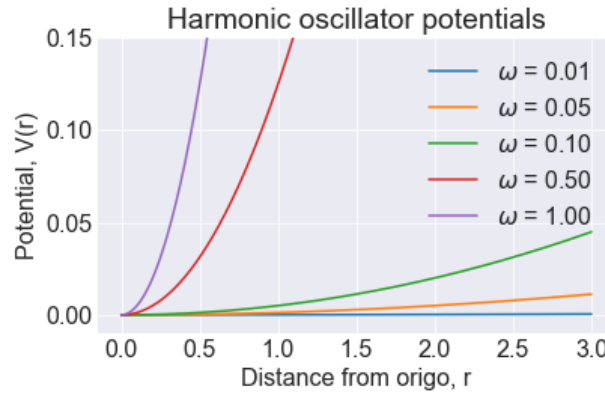


Figure 2: •

3 Results and discussion

3.1 Two electrons in two dimensions

3.1.1 Brute force sampling

Standard error of the mean (SEM):

$$\text{SEM} = \frac{\sigma}{\sqrt{N}} \quad (9)$$

where N is the number of observations, in our case the number of Monte Carlo cycles.

Table 2: Comparing the results for analytical/numerical evaluation of the double derivative. Energy are in atomic units (a.u.) and CPU time is in units of seconds.

Analytical:					Numerical:				
α :	$\langle E_L \rangle$:	SEM:	σ_B :	CPU time:	α :	$\langle E_L \rangle$:	SEM:	σ_B :	CPU time:
0.50	2.49402	0.00073	0.01022	5.57812	0.50	2.49991	0.00073	0.01093	18.20310
0.60	2.26441	0.00052	0.00690	5.76562	0.60	2.26412	0.00053	0.00727	18.21880
0.70	2.13118	0.00035	0.00448	5.92188	0.70	2.13039	0.00036	0.00436	18.62500
0.80	2.05016	0.00022	0.00263	5.67188	0.80	2.04993	0.00022	0.00269	18.46880
0.90	2.01015	0.00010	0.00116	5.96875	0.90	2.01160	0.00010	0.00118	18.46880
1.00	2.00000	0.00000	0.00000	5.62500	1.00	2.00000	0.00000	0.00000	18.31250
1.10	2.00871	0.00009	0.00102	6.20312	1.10	2.00825	0.00009	0.00097	18.35940
1.20	2.03402	0.00018	0.00175	6.34375	1.20	2.03308	0.00018	0.00170	18.31250
1.30	2.07259	0.00026	0.00244	5.95312	1.30	2.06460	0.00026	0.00243	20.23440
1.40	2.11041	0.00034	0.00311	6.15625	1.40	2.11803	0.00033	0.00308	19.00000
Mean CPU time: 5.91875					Mean CPU time: 18.62033				

3.1.2 Including importance sampling

Table 3: Comparing the results for importance/brute force sampling. Energy are in atomic units (a.u.) and CPU time is in units of seconds. Here the parameter α is set to 0.9.

	Brute force:					Importance:				
dl :	$\langle E_L \rangle$:	SEM:	σ_B :	Acc.:	t_{CPU} :	$\langle E_L \rangle$:	SEM:	σ_B :	Acc.:	t_{CPU} :
1.000	2.011	0.00010	0.00068	79.834	6.125	2.016	0.00012	0.00027	68.528	8.453
0.500	2.010	0.00010	0.00118	89.814	5.812	1.987	0.00011	0.00026	82.230	8.625
0.100	2.013	0.00010	0.00496	97.951	5.859	2.005	0.00011	0.00051	97.874	8.203
0.050	2.003	0.00010	0.00860	98.995	5.656	2.012	0.00011	0.00070	99.358	7.875
0.010	2.004	0.00010	0.02281	99.798	6.188	2.011	0.00010	0.00145	99.967	7.984
0.005	1.948	0.00004	0.01005	99.909	6.359	2.011	0.00010	0.00214	99.992	7.656
0.001	2.018	0.00001	0.00211	99.980	6.094	2.015	0.00011	0.00487	99.999	7.703
	Mean CPU time: 6.01339					Mean CPU time: 8.07143				

3.1.3 Including optimization

Minimization rate of 0.5 seemed to be ideal.

3.1.4 Including interaction

Table 4: •

ω	α	β	$\langle E_L \rangle$	SEM	σ_B	$ \mathbf{r}_1 - \mathbf{r}_2 _{mean}$	$\langle T \rangle$	$\langle V_{ext} \rangle$	$\langle V_{int} \rangle$
1.0	0.98834	0.39975	3.00695	0.00002	0.00013	1.63102	0.902159	1.291000	0.813795
0.5	0.48521	0.34998	2.00632	0.00002	0.00022	2.43018	0.788484	0.689334	0.52850
0.1	0.07937	0.17917	1.67700	0.00003	0.00068	7.31240	1.310000	0.210041	0.156958

3.2 Extending to more particles

3.2.1 Six particles

3.2.2 Twelve particles

Appendices

A Iteration - derivatives with regards to parameters

$$\frac{\partial \psi_T}{\partial \alpha} = -\frac{\omega}{2} \sum_i^N r_i^2 \quad (10)$$

$$\frac{\partial \psi_T}{\partial \beta} = -\sum_{i < j}^N \frac{a_{ij} r_{ij}^2}{(1 + \beta r_{ij})^2} \quad (11)$$

B Dealing with the Slater determinant efficiently

Determining a determinant numerically is a costly operation, so we want to do some alteration to increase the efficiency of the code.

B.1 Slater determinant

The Slater determinant contains the single-particle wave function of the number of particles included in the system evaluated at the position for all particles included because electrons are indistinguishable. The determinant is written as

$$D = \text{Det}(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_N(\mathbf{r}_N)) = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) & \cdots & \phi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N) & \phi_2(\mathbf{r}_N) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix}$$

Hence the rows represent different positions, r_i , and the columns represent different states. To simplify the calculations we want to have all states with spin up in one determinant and all states with spin down in another determinant. For six particles we then get

$$D = D_{\uparrow} D_{\downarrow} = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_3(\mathbf{r}_1) & \phi_5(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_3(\mathbf{r}_2) & \phi_5(\mathbf{r}_2) \\ \phi_1(\mathbf{r}_3) & \phi_3(\mathbf{r}_3) & \phi_5(\mathbf{r}_3) \end{vmatrix} \begin{vmatrix} \phi_2(\mathbf{r}_4) & \phi_4(\mathbf{r}_4) & \phi_6(\mathbf{r}_4) \\ \phi_2(\mathbf{r}_5) & \phi_4(\mathbf{r}_5) & \phi_6(\mathbf{r}_5) \\ \phi_2(\mathbf{r}_6) & \phi_4(\mathbf{r}_6) & \phi_6(\mathbf{r}_6) \end{vmatrix}.$$

We see this from Tab. 1 and Eq. 3. *Mister anti-symmetrien, men expectation value er lik.*

The trial wavefunction can therefore be rewritten to

$$\psi_T = D_{\uparrow} D_{\downarrow} \psi_C$$

where ψ_C is the correlation part of the trial wavefunction. Now we only have to update one of these matrices when we move a particle, depending on which spin the particle has.

B.2 The Metropolis ratio

In the metropolis test we calculate the ratio between the wavefunction before and after a proposed move, but now the wavefunction includes a determinant which is costly to calculate. We therefore want to utilize some relations from linear algebra to simplify the ratio and make the algorithm more efficient. The ratio between the Slater determinant part of the wavefunction, ψ_{SD} , is

$$R = \frac{\psi_{SD}(\mathbf{r}^{new})}{\psi_{SD}(\mathbf{r}^{old})} = \frac{\sum_i^N d_{ij}(\mathbf{r}^{new}) C_{ij}(\mathbf{r}^{new})}{\sum_i^N d_{ij}(\mathbf{r}^{old}) C_{ij}(\mathbf{r}^{old})}. \quad (12)$$

where $d_{ij} = \psi_i(j)$

Here we have used the fact that when you calculate a determinant, you break it down into a sum of smaller determinants times a factor:

$$D = \begin{vmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ d_{21} & d_{22} & \cdots & d_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ d_{N1} & d_{N2} & \cdots & d_{NN} \end{vmatrix} = \sum_i^N d_{ij} C_{ij}.$$

So if $d_{ij} = d_{11}$ then

$$C_{11} = \begin{vmatrix} d_{22} & d_{23} & \cdots & d_{2N} \\ d_{32} & d_{33} & \cdots & d_{3N} \\ \vdots & \vdots & \ddots & \vdots \\ d_{N2} & d_{N3} & \cdots & d_{NN} \end{vmatrix}.$$

We observe in Eq. 12 that if we move particle j from r_j^{old} to r_j^{new} the matrix C_{ij} is unchanged, we have only changed the d_{ij} in the original determinant D that is not included in C_{ij} . Equation 12 is

then

$$R = \frac{\sum_i^N d_{ij}(\mathbf{r}^{new})}{\sum_i^N d_{ij}(\mathbf{r}^{old})} \quad (13)$$

We can simplify this even further with the relation

$$\sum_{k=1}^N d_{ik} d_{kj}^{-1} = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \quad (14)$$

The ratio can be rewritten as

$$R = \frac{\sum_i^N d_{ij}(\mathbf{r}^{new}) d_{ij}(\mathbf{r}^{old})^{-1}}{\sum_i^N d_{ij}(\mathbf{r}^{old}) d_{ij}(\mathbf{r}^{old})^{-1}} = \sum_i^N d_{ij}(\mathbf{r}^{new}) d_{ij}(\mathbf{r}^{old})^{-1}. \quad (15)$$

The consequence of these calculations are that we now only have to calculate the invers values of the determinant once to know the values for $d_{ij}(\mathbf{r}^{old})^{-1}$ and then update only the row of the position that was changed in the Slater determinant and calculate the invers of the determinant again only if the move is accepted.

B.3 Updating the inverse of the Slater determinant

After a move is accepted in the Metropolis test, the row in the Slater determinant representing that particle is updated, but the inverse of the Slater determinant also needs to be updated because the Slater determinant has changed. This could be done by simply calculating the inverse of the determinant, but this is costly and there is a more efficient way. The elements of the determinant d_{kj}^{-1} (hva betyr den $^{-1}$? At den skal opphøyes i minus 1 eller er det notasjon på at det er et element i den inverse matrisen?) can be found through

$$d_{kj}^{-1}(\mathbf{r}^{new}) = \begin{cases} d_{kj}^{-1}(\mathbf{r}^{old}) - \frac{d_{kj}^{-1}(\mathbf{r}^{old})}{R} \sum_{l=1}^N d_{il}^{-1}(\mathbf{r}^{new}) d_{lj}^{-1}(\mathbf{r}^{old}) & \text{if } i \neq j \\ \frac{d_{kj}^{-1}(\mathbf{r}^{old})}{R} \sum_{l=1}^N d_{il}^{-1}(\mathbf{r}^{old}) d_{lj}^{-1}(\mathbf{r}^{old}) & \text{if } i = j \end{cases},$$

where i is the number of the row representing the particle that was moved.

C Energies

$$E_{n_x n_y} = \hbar \omega (n_x + n_y + \frac{d}{2}) \quad (16)$$

where d is the number of dimensions. In this project $d = 2$.

Table 5: The exact energies for the non-interacting case with different number of particles in a closed shell system.

Energies	
E_{00}	$\hbar\omega$
$E_{10} = E_{01}$	$2\hbar\omega$
$E_{20} = E_{02} = E_{11}$	$3\hbar\omega$
$E_{30} = E_{03} = E_{21} = E_{12}$	$4\hbar\omega$
$E_{N=2} = 2E_{00}$	$2\hbar\omega$
$E_{N=6} = E_{N=2} + 2E_{10} + 2E_{01}$	$10\hbar\omega$
$E_{N=12} = E_{N=6} + 2E_{20} + 2E_{02} + 2E_{11}$	$28\hbar\omega$
$E_{N=20} = E_{N=12} + 2E_{30} + 2E_{03} + 2E_{21} + 2E_{12}$	$60\hbar\omega$

D Hermite polynomials and the wavefunction derivatives

The relevant Hermite polynomials

$H_0(\sqrt{\omega}x)$	1
$H_1(\sqrt{\omega}x)$	$2\sqrt{\omega}x$
$H_2(\sqrt{\omega}x)$	$4\omega x^2 - 2$
$H_3(\sqrt{\omega}x)$	$8\omega\sqrt{\omega}x^3 - 12\sqrt{\omega}x$

$$\phi_{n_x, n_y}(x, y) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp(-\omega(x^2 + y^2)/2).$$

Table 6: $\psi_{n_x n_y}$

Trial wavefunctions for the different states

ψ_{00}	$A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{01}	$2\sqrt{\omega}x A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{10}	$2\sqrt{\omega}y A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{20}	$(4\omega x^2 - 2) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{02}	$(4\omega y^2 - 2) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{11}	$4\omega xy A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{30}	$(8\omega\sqrt{\omega}x^3 - 12\sqrt{\omega}x) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{03}	$(8\omega\sqrt{\omega}y^3 - 12\sqrt{\omega}y) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{21}	$(8\omega\sqrt{\omega}x^2y - 4\sqrt{\omega}y) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
ψ_{12}	$(8\omega\sqrt{\omega}xy^2 - 4\sqrt{\omega}x) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$

Table 7: $\psi_{n_x n_y}$

The derivative of the trial wavefunctions for the different states

$\nabla \psi_{00}$	$(-\alpha \omega x, -\alpha \omega y) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{01}$	$-(\sqrt{\omega}(a\omega x^2 - 1), \alpha \omega^{3/2}xy) 2A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{10}$	$-(\alpha \omega^{3/2}xy, \sqrt{\omega}(a\omega y^2 - 1)) 2A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{20}$	$-(2\alpha \omega^2 x^3 - \alpha \omega x - 4\omega x, 2\alpha \omega^2 x^2 y - \alpha \omega y) 2A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{02}$	$-(2\alpha \omega^2 xy^2 - \alpha \omega x, 2\alpha \omega^2 y^3 - \alpha \omega y - 4\omega y) 2A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{11}$	$(-4\omega y(\alpha \omega x^2 - 1), -4\omega x(\alpha \omega y^2 - 1)) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{30}$	$(-4\sqrt{\omega}(2\alpha \omega^2 x^4 - 3(\alpha + 2)\omega x^2 + 3), -4\alpha \omega^{3/2}xy(2\omega x^2 - 3)) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{03}$	$(-4\sqrt{\omega}(-4\alpha \omega^{3/2}xy(2\omega y^2 - 3), 2\alpha \omega^2 y^4 - 3(\alpha + 2)\omega y^2 + 3)) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{21}$	$(-4\sqrt{\omega}(\alpha \omega x^2(2\omega xy - 1) - 4\omega xy + 1), -4\omega^{3/2}x(2x(\alpha \omega y^2 - 1) - \alpha y)) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla \psi_{12}$	$(-4\omega^{3/2}y(2y(\alpha \omega x^2 - 1) - \alpha x), -4\sqrt{\omega}(\alpha \omega y^2(2\omega xy - 1) - 4\omega xy + 1)) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$

Table 8: $\psi_{n_x n_y}$

The double derivative of the trial wavefunctions for the different states

$\nabla^2 \psi_{00}$	$(\alpha^2 \omega^2 r^2 - \alpha \omega) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{01}$	$2\alpha \omega^{3/2} x (\alpha \omega r^2 - 4) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{10}$	$2\alpha \omega^{3/2} y (\alpha \omega r^2 - 4) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{20}$	$2\omega (\alpha^2 \omega (2\omega x^2 - 1) r^2 + \alpha (2 - 12\omega x^2) + 4) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{02}$	$2\omega (\alpha^2 \omega (2\omega y^2 - 1) r^2 + \alpha (2 - 12\omega y^2) + 4) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{11}$	$4\alpha \omega^2 xy (\alpha \omega r^2 - 6) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{30}$	$4\omega^{3/2} x (\alpha^2 \omega (2\omega x^2 - 3) r^2 - 4\alpha (4\omega x^2 - 3) + 12) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{03}$	$4\omega^{3/2} y (\alpha^2 \omega (2\omega y^2 - 3) r^2 - 4\alpha (4\omega y^2 - 3) + 12) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{21}$	$4\omega^{3/2} (\alpha^2 \omega x r^2 (2\omega xy - 1) + 4\alpha x (1 - 4\omega xy) + 4y) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$
$\nabla^2 \psi_{12}$	$4\omega^{3/2} (\alpha^2 \omega y r^2 (2\omega xy - 1) + 4\alpha y (1 - 4\omega xy) + 4x) A \exp \left(\frac{-\alpha \omega r^2}{2} \right)$

References

- [1] Vilde M Reinertsen. Project 1, 2020.