Project 2

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Abstract

This is the abstract.

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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

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

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

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

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 $a_0 =$ ... and the unit of energy is .... We also have $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$ 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

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

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.

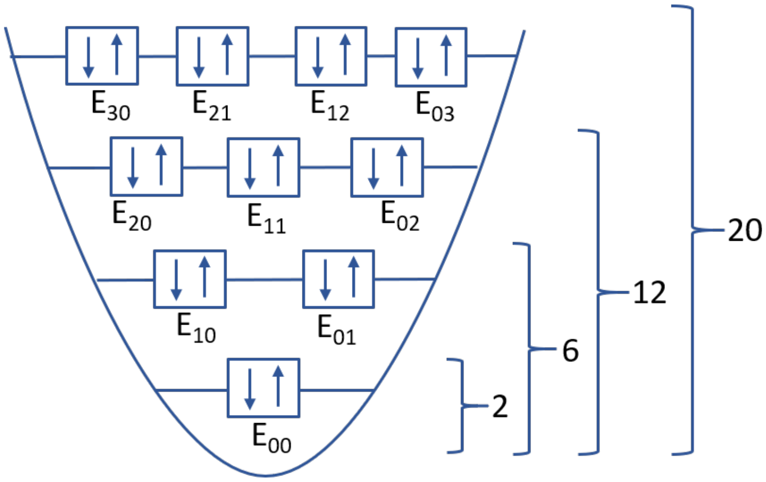

Figure 1: •

The expectation value can be found by solving the equation

$$\langle E\rangle = \frac{\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \psi_T^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\hat{H}(\boldsymbol{r}_1,\boldsymbol{r}_2)\psi_T(\boldsymbol{r}_1,\boldsymbol{r}_2)}{\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \psi_T^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\psi_T(\boldsymbol{r}_1,\boldsymbol{r}_2)}. \tag{3}$$

We will use Variational Monte Carlo (VMC) methods to evaluate the Eq. 3. The exact wave function for two not interacting electrons in the ground state is given by

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

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

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

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

$$\psi_T(\boldsymbol{r}_1,\boldsymbol{r}_2) = C\exp\left(-\alpha\omega(r_1^2+r_2^2)/2\right)\exp\left(\frac{ar_{12}}{(1+\beta r_{12})}\right), \tag{4}$$

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

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_6) = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_6(\boldsymbol{r}_6)\right) \prod_{i<j}^{6} \exp\left(\frac{a r_{ij}}{(1 + \beta r_{ij})}\right), \tag{5}$$

where

$$Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_6(\boldsymbol{r}_6)\right) = \begin{vmatrix} \phi_1(\boldsymbol{r}_1) & \phi_2(\boldsymbol{r}_1) & \cdots & \phi_6(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_2(\boldsymbol{r}_2) & \cdots & \phi_6(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r}_6) & \phi_2(\boldsymbol{r}_6) & \cdots & \phi_6(\boldsymbol{r}_6) \end{vmatrix}$$

is the Slater determinant. This determinant occurs because electron are indistinguishable particles and they are antisymmetric ... . The functions, $\phi_i(\boldsymbol{r}_j)$, are given by Eq. 2 and the notation is explained in Tab. 1.

Table 1: The relation between the notation used in the determinant (left) compared to Eq. 2 (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

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_{12}) = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_{12}(\boldsymbol{r}_{12})\right) \prod_{i<j}^{12} \exp\left(\frac{a r_{ij}}{(1 + \beta r_{ij})}\right). \tag{6}$$

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 spactial 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 devide 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. But how is it done? Is it foreces like I have done it now?*

2.4 Virial theorem

Explain.

$$2 \langle T \rangle = - \langle V_{ext} \rangle \tag{7}$$

3 Results and discussion

3.1 Two electrons in two dimensions

3.1.1 Ground state with no interaction

3.1.2 Including importance sampling

3.1.3 Including optimization

3.1.4 Including interaction

3.2 Extending to more particles

3.2.1 Six particles

3.2.2 Twelve particles

Appendices

A Iteration - derivatives with regards to parameters

$$\frac{\partial \psi_T}{\partial \alpha} = -\frac{\omega}{2} \sum_i^N r_i^2 \tag{8}$$

$$\frac{\partial \psi_T}{\partial \beta} = - \sum_{i<j}^N \frac{a_{ij} r_{ij}^2}{(1 + \beta r_{ij})^2} \tag{9}$$

B Dealing with the Slater determinant efficiently

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

B.1 Slater determinant

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

$$D = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_N(\boldsymbol{r}_N)\right) = \begin{vmatrix} \phi_1(\boldsymbol{r}_1) & \phi_2(\boldsymbol{r}_1) & \cdots & \phi_N(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_2(\boldsymbol{r}_2) & \cdots & \phi_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r}_N) & \phi_2(\boldsymbol{r}_N) & \cdots & \phi_N(\boldsymbol{r}_N). \end{vmatrix}$$

Hence the rows represent different positions, r_i, and the coloumns represent different states. To simplify the calcualtions 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

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

We see this from Tab. 1 and Eq. 2. *Mister anti-symmertrien, 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 matrises 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 bewteen 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 efficent. The ratio between the Slater determinant part of the wavefunction, ψ_{SD}, is

$$R = \frac{\psi_{SD}(\boldsymbol{r}^{new})}{\psi_{SD}(\boldsymbol{r}^{old})} = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new}) C_{ij}(\boldsymbol{r}^{new})}{\sum_i^N d_{ij}(\boldsymbol{r}^{old}) C_{ij}(\boldsymbol{r}^{old})}. \tag{10}$$

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 $dij = d_{11}$ 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. 10 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 10 is then

$$R = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new})}{\sum_i^N d_{ij}(\boldsymbol{r}^{old})} \tag{11}$$

We can simplify this even further with the relation

$$\sum_{k=1}^N d_{ik} d_{kj}^{-1} = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \tag{12}$$

The ratio can be rewritten as

$$R = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new}) d_{ij}(\boldsymbol{r}^{old})^{-1}}{\sum_i^N d_{ij}(\boldsymbol{r}^{old}) d_{ij}(\boldsymbol{r}^{old})^{-1}} = \sum_i^N d_{ij}(\boldsymbol{r}^{new}) d_{ij}(\boldsymbol{r}^{old})^{-1}. \tag{13}$$

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 $d_{ij}(\boldsymbol{r}^{old})^{-1}$ 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

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

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

C Energies

$$E_{n_x n_y} = \hbar\omega(n_x + n_y + \frac{d}{2}) \tag{14}$$

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

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

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

Table 3: $\psi_{n_x n_y}$

Trial wavefunctions for the different states	
ψ_{00}	$A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{01}	$2\sqrt{\omega}xA\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{10}	$2\sqrt{\omega}yA\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
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}	$4\omega xyA\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
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 4: $\psi_{n_x n_y}$

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

Table 5: $\psi_{n_x n_y}$

The double derivative of the trial wavefunctions for the different states	
$\nabla^2\psi_{00}$	$(\alpha^2\omega^2 r^2 - \alpha\omega)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{01}$	$2\alpha\omega^{3/2}x(\alpha\omega r^2 - 4)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{10}$	$2\alpha\omega^{3/2}y(\alpha\omega r^2 - 4)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{20}$	$2\omega(\alpha^2\omega(2\omega x^2 - 1)r^2 + \alpha(2 - 12\omega x^2) + 4))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{02}$	$2\omega(\alpha^2\omega(2\omega y^2 - 1)r^2 + \alpha(2 - 12\omega y^2) + 4))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{11}$	$4\alpha\omega^2 xy(\alpha\omega r^2 - 6)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{30}$	$4\omega^{3/2}x(\alpha^2\omega(2\omega x^2 - 3)r^2 - 4\alpha(4\omega x^2 - 3) + 12)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{03}$	$4\omega^{3/2}y(\alpha^2\omega(2\omega y^2 - 3)r^2 - 4\alpha(4\omega y^2 - 3) + 12)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{21}$	$4\omega^{3/2}(\alpha^2\omega x r^2(2\omega xy - 1) + 4\alpha x(1 - 4\omega xy) + 4y)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{12}$	$4\omega^{3/2}(\alpha^2\omega y r^2(2\omega xy - 1) + 4\alpha y(1 - 4\omega xy) + 4x)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$