Project 2

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Abstract

This is the abstract.

Contents

1 Introduction

2 Theory and method

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

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

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

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

The functions $H_{n_x}(\sqrt{\omega}x)$ are so-called Hermite polynomials, discussed in connection with project 1 while A is a normalization constant. For the lowest-lying state we have $n_x = n_y = 0$ and an energy $\epsilon_{n_x,n_y} = \omega(n_x + n_y + 1) = \omega$. Convince yourself that the lowest-lying energy for the two-electron system is simply 2ω.

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

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

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

$r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ (with $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$)

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_6) = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \dots, \phi_6(\boldsymbol{r}_6)\right) \prod_{i<j}^{6} \exp\left(\frac{ar_{ij}}{(1+\beta r_{ij})}\right), \tag{4}$$

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_{12}) = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \dots, \phi_{12}(\boldsymbol{r}_{12})\right) \prod_{i<j}^{12} \exp\left(\frac{ar_{ij}}{(1+\beta r_{ij})}\right), \tag{5}$$

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 Dealing with the Slater determinant efficiently

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

$$R = \frac{\psi_{SD}(\boldsymbol{r}^{new})}{\psi_{SD}(\boldsymbol{r}^{old})} = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new})C_{ij}(\boldsymbol{r}^{new})}{\sum_i^N d_{ij}(\boldsymbol{r}^{old})C_{ij}(\boldsymbol{r}^{old})}. \tag{6}$$

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. 6 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 6 is then

$$R = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new})}{\sum_i^N d_{ij}(\boldsymbol{r}^{old})} \tag{7}$$

We can simplify this even further with the relation

$$\sum_{k=1}^{N} d_{ik} d_{kj}^{-1} = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \tag{8}$$

The ratio can be rewritten as

$$R = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new}) d_{ij}(\boldsymbol{r}^{old})^{-1}}{\sum_i^N d_{ij}(\boldsymbol{r}^{old}) d_{ij}(\boldsymbol{r}^{old})^{-1}} = \sum_i^N d_{ij}(\boldsymbol{r}^{new}) d_{ij}(\boldsymbol{r}^{old})^{-1}. \tag{9}$$

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 the row that is changed if the move is accepted.

B Energies

$$E_{n_x n_y} = \hbar\omega(n_x + n_y + \frac{d}{2}) \tag{10}$$

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

Table 1: The exact energies for the non-interacting case with different number of particles in a closed shell system.

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

C Hermite polynomials 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 2: $\psi_{n_x n_y}$

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 3: $\psi_{n_x n_y}$

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 4: $\psi_{n_x n_y}$

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