Fys4110: Project 2

Knut Halvor Helland

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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. I have collected the differentiations here. Trial wave function is

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

A.1 Gradient

In order to compute the driftforce for importance sampling we needed

$$\frac{1}{\psi_T}\frac{\mathrm{d}\psi_T}{\mathrm{d}z},$$

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

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

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

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

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

$$
\begin{aligned}
\frac{1}{\psi_T}\frac{\partial^2\psi_T}{\partial z_i^2} &= \frac{\partial^2}{\partial z_i^2}\left(-\alpha\omega(r_1^2+r_2^2)/2+\frac{ar_{12}}{1+\beta r_{12}}\right)+\left(\frac{\partial}{\partial z_i}\left(-\alpha\omega(r_1^2+r_2^2)/2+\frac{ar_{12}}{1+\beta r_{12}}\right)\right)^2 \\
&= \frac{\partial}{\partial z_i}\left(-\alpha\omega z_i+\frac{a}{(1+\beta r_{12})^2}\frac{(z_i-z_j)}{r_{12}}\right)+\left(-\alpha\omega z_i+\frac{a}{(1+\beta r_{12})^2}\frac{(z_i-z_j)}{r_{12}}\right)^2 \\
&= -\alpha\omega+\frac{a}{(1+\beta r_{12})^2 r_{12}}-\frac{2a\beta(z_i-z_j)^2}{(1+\beta r_{12})^3 r_{12}^2}-\frac{a(z_i-z_j)^2}{(1+\beta r_{12})^2 r_{12}^3}+\alpha^2\omega^2 z_i^2-\frac{2\alpha\omega a z_i(z_i-z_j)}{(1+\beta r_{12})^2 r_{12}}+\frac{a^2(z_i-z_j)^2}{(1+\beta r_{12})^4 r_{12}^2}.
\end{aligned}
$$

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.

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

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