Fys4110: Project 2

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Abstract

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

3 Trial wave functions

3.1 2 Particle Case

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

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

with α and β as free parameters.

3.2 Slater case

For the many particle case we will use the non-interacting ground state Slater determinant for a modified potential of strength $\alpha\omega$ 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 too complicated too do in

our timeframe. Instead we will compare the Hartree-Fock approach to adding a Jastrow factor to this modified ground state.

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

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:

$$\psi_T = \mathcal{A}\left(\psi_{1,\downarrow}(\alpha)\dots\psi_{N/2,\downarrow}(\alpha);\boldsymbol{r}_1\dots\boldsymbol{r}_{N/2}\right)\mathcal{A}\left(\psi_{1\uparrow}(\alpha)\dots\psi_{N/2\uparrow}(\alpha);\boldsymbol{r}_{N/2+1}\dots\boldsymbol{r}_N\right)\prod_{i<j}^{N}\exp\left(-\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right). \tag{4}$$

In the 2 particle case this reduces to equation 2.

4 Monte-Carlo Integration

In this project I will estimate the energy of the trial wavefunctions with Monte-Carlo (MC) integration. MC integration is a method of estimating the value of integrals on the form

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

where $p(x_1,\dots,x_N)$ is a probability density function. MC integration is then based on drawing points $\boldsymbol{r}_i$ according to p and evaluating F in these points

$$F_i \equiv F(\boldsymbol{r}_i). \tag{6}$$

Then defining

$$\overline{F} \equiv \frac{1}{N}\sum_{i=1}^{N}F_i \tag{7}$$

we have that

$$\langle F\rangle = \lim_{N\to\infty}\overline{F}. \tag{8}$$

Since we cannot draw infinite points we use $\overline{F}$ as an estimate of $\langle F\rangle$.

In order to estimate an integral in this way we thus need a method to draw positions according to p, a way to compute F_i and a way to estimate the error in the integration.

4.1 The Metropolis Algorithm

The Metropolis algorithm is a way to draw points according to a probability ensity function p. It is based on semi randomly-walking through the space. One advantage of the method is that the pdf does not need to be normalised, which is convenient. We can thus rewrite equation 5 to

$$\langle F\rangle = \frac{\int F(x_1,\dots,x_N)p(x_1,\dots,x_N)\prod_{k=1}^{N}\mathrm{d}x_k}{\int p(x_1,\dots,x_N)\prod_{k=1}^{N}\mathrm{d}x_k}. \tag{9}$$

One disadvantage is that as the each point is only a relatively small step from the last the correlations between points are high enough that we have to take them into account.

4.1.1 Detailed Balance

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

$$P(a)P(b|a) = P(b)P(a|b), \tag{10}$$

or rewritten

$$\frac{P(a)}{P(b)} = \frac{P(a|b)}{P(b|a)}. \tag{11}$$

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

$$\frac{A(a|b)}{A(b|a)} = \frac{P(a)G(b|a)}{P(b)G(a|b)}. \tag{12}$$

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

$$A(a|b) = \min\left(1, \frac{P(a)G(b|a)}{P(b)G(a|b)}\right). \tag{13}$$

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 13.
3. Draw a random number $0 \leq r < 1$ from a uniform distribution.
4. If $a > r$ accept the move. Else reject the move.
5. Save position
6. return to point 1.

4.1.2 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.

4.1.3 Importance Sampling

If we instead choose a non-symmetric proposal distribution we may choose one to maximise the acceptancerate. If we choose a proposal distribution 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 $G(a|b) > G(b|a)$, we will increase the acceptance rate. We need to make sure that the proposal distribution preserves ergodicity, which means that the whole space may be reached from any point with enought steps. So the probability of proposing a move into an area with lower probability must be non-zero. The obvious way to ensure proposals into higher probability is to use the gradient of p:

$$\frac{1}{p}\nabla p = \frac{1}{|\psi_T|^2}\nabla|\psi|^2 = \frac{2}{\psi_T}\nabla\psi \equiv 2F, \tag{14}$$

where I have used that the wavefunction is real. If we only move one particle at a time in one direction at a time we only the derivative with respect to that particle in that dimension. One choice that uses this and preserves ergodicity is

$$\boldsymbol{x}_{i,n+1} = \boldsymbol{x}_{i,n} + \sigma\chi + \sigma^2 F(x_{i,n}), \tag{15}$$

where χ is a random variable from a gaussian distribution about 0 with standard deviation 1. From [4] the proposal distribution from this rule is

$$G(x_{i,n+1}|x_{i,n}) = \exp\left(-\frac{(x_{i,n+1} - x_{i,n} - \sigma^2 F(x_{i,n}))^2}{2\sigma^2}\right). \tag{16}$$

4.2 Local Energy

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

$$\langle O \rangle = \frac{\int \psi^* O \psi \prod_i \mathrm{d}x_i}{\int |\psi|^2 \prod_i \mathrm{d}x_i}, \tag{17}$$

This is not exactly on the form of equation 9, but it can be rewritten in terms of local variables given by

$$O_L = \frac{1}{\psi} O\psi, \tag{18}$$

so that the expectation value is

$$\langle O \rangle = \frac{\int |\psi|^2 O_L \prod_i \mathrm{d}x_i}{\int |\psi|^2 \prod_i \mathrm{d}x_i}. \tag{19}$$

So the expectation value of the energy is given by

$$\langle E \rangle = \frac{\int |\psi|^2 E_L \prod_i \mathrm{d}x_i}{\int |\psi|^2 \prod_i \mathrm{d}x_i}, \tag{20}$$

with

$$E_L = \frac{1}{\psi} H\psi, . \tag{21}$$

4.2.1 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

$$E_L(\boldsymbol{r_1}, \boldsymbol{r_2}) = \left[\frac{1}{2}(1-\alpha)\omega(r_1^2 + r_2^2) + 2\alpha\omega\right] - \frac{a}{(1+\beta r_{12})^2}\left[\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1+\beta r_{12})} - \alpha\omega r_{12}\right] + \frac{1}{r_{12}}, \tag{22}$$

as shown in appendix B.2.

4.2.2 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

4.3 Error Estimation and Blocking

In this section I follow [2] and [4] in explaining the blocking method. Let $\{ F_i \}$ be a finite set of consecutive measurements of the quantity F on a system in equilibrium, in other words the probability distribution for the measurements is independent of time. Then as above the average of $\{ F_i \}$ $\overline{F}$ is an estimate of the true average of F $\langle F \rangle$. An estimate of the error in this aproximation is given by the standard deviation of $\overline{F}$ $\sigma_{\overline{F}}$. The variance in $\overline{F}$ is given by

$$\sigma_{\overline{F}}^2 = \left\langle \overline{F}^2 \right\rangle - \left\langle \overline{F} \right\rangle^2, \tag{23}$$

expanding this we find

$$\begin{aligned}\sigma_{\overline{F}}^2 &= \left\langle \left(\frac{1}{N} \sum_{i=1}^{N} F_i \right)^2 \right\rangle - \left\langle \frac{1}{N} \sum_{i=1}^{N} F_i \right\rangle^2 \\ &= \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\langle F_i F_j \rangle - \langle F_i \rangle \langle F_j \rangle \right) \\ &= \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \operatorname{cov}(F_i, F_j).\end{aligned}$$

The time independence of the pdf means that the covariance should only depend on the relative distance between i and j $t \equiv |i-j|$. So we can define $C(t) = \operatorname{cov}(F_i, F_j)$. Now we can split $\sigma_{\overline{F}}^2$ into

$$\sigma_{\overline{F}}^2 = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} C(t(i,j)) = \frac{1}{N} \left[C(0) + 2 \sum_{t=0}^{N-1} \left(1 - \frac{t}{N} \right) C(t) \right] \tag{24}$$

For uncorrelated data $C(t > 0) = 0$ so the standard deviation of the error is $\sigma_F / \sqrt{N}$, which is easy to estimate. With corelations things are more complicated, however the blocking method allows us to incorperate correlations into a similar calculation. If we transform the data set $\{ F_i \}$ into another set $\{ \tilde{F}_i \}$, where

$$\tilde{F}_i = \frac{1}{B} \sum_{j=1}^{B} F_{(i-1)B+j}, \tag{25}$$

where B is a whole number called the block size. Call $\tilde{F}_i$ a block. Expanding $\tilde{C}(0)$ we see that

$$\begin{aligned}\tilde{C}(0) &= \left\langle \tilde{F}_i^2 \right\rangle - \left\langle \tilde{F}_i \right\rangle^2 \\ &= \frac{1}{B^2} \sum_{a,b}^{B} \left\langle \tilde{F}_{i+a} \tilde{F}_{i+b} \right\rangle - \left\langle \tilde{F}_{i+a} \right\rangle \left\langle \tilde{F}_{i+b} \right\rangle \\ &= \frac{1}{B^2} \sum_{a,b}^{B} C(|a-b|) \\ &= \frac{1}{B} \sum_{t=0}^{B-1} C(t),\end{aligned}$$

and so

$$\frac{\tilde{C}(0)}{N/B} = \frac{1}{N} \left[C(0) + \sum_{t=1}^{B-1} C(t) \right], \tag{26}$$

comparing with equation 24 we see that blocking has incorporated part of the error from correlations into $\tilde{C}(0)$, which is just as easy to estimate as $C(0)$. So, for an appropriate block size an improved estimate of the error is approximated by

$$\sigma_{\overline{F}}^2 \approx \frac{\left(\overline{\tilde{F}^2} - \overline{\tilde{F}}^2 \right)}{N/B - 1}. \tag{27}$$

To find the approriate block size we may plot this estimate as a function of block size, and choose a value where this seems to flatten.

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 A Note About Cofactors and Determinants

Determinants can be somewhat hard to work with, following [4] we may use cofactors to do some trickery. For a matrix A with elements A_{ij} the cofactors C_{ij} are given by $(-1)^{i+j}M_{ij}$, with M_{ij} being the determinant of the matrix formed by deliting the ith row and jth collumn from A. There two properties of cofactors that will be important here are

$$|A|\mathbf{1} = AC^T \Leftrightarrow |A| = \sum_j A_{ij}C_{ij}, \tag{28}$$

and thus

$$A^{-1} = \frac{1}{|A|}C^T \Leftrightarrow A^{-1}_{ij} = \frac{1}{|A|}C_{ji}, \tag{29}$$

and the fact that C_{ij} is independent of row i and collumn j of A.

B 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.

B.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 $z_i = x_2$, $z_j = x_1$.

B.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

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

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

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.

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

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

C 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.

C.1 Gradient

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

$$\frac{1}{\psi_T}\frac{\partial \psi_T}{\partial z_i} = \frac{1}{|s|}\frac{\partial |s|}{\partial z_i} + \frac{1}{J}\frac{\partial J}{\partial z_i}.$$

For the derivative of the determinant we exploit the properties noted in section A to see that

$$\frac{1}{|s|}\frac{\partial |s|}{\partial z_i} = \frac{1}{|s|}\sum_j \frac{\partial s_{ij}}{\partial z_i} C_{ij},$$

since C_{ij} is independent of z_i. Rewriting $C_{ij} = |s| s_{ji}^{-1}$ we find

$$\frac{1}{|s|}\frac{\partial |s|}{\partial z_i} = \sum_j \frac{\partial s_{ij}}{\partial z_i} s_{ji}^{-1}.$$

From section B.1 it is clear that

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

so

$$\frac{1}{\psi_T}\frac{\partial \psi_T}{\partial z_i} = \sum_j \frac{\partial s_{ij}}{\partial z_i} s_{ji}^{-1} + \sum_{j\neq i} \frac{a_{ij}}{(1+\beta r_{ij})^2}\frac{(z_i - z_j)}{r_{ij}}.$$

C.2 Laplacian

Writing $\psi_T = \psi_S J$ we can write the Laplacian as

$$\frac{\nabla^2 \psi_T}{\psi_T} = \frac{\nabla^2 \psi_S}{\psi_S} + \frac{\nabla^2 J}{J} + 2\frac{\nabla \psi_S}{\psi_S}\cdot\frac{\nabla J}{J},$$

expanding the Slater part $\psi_S = |S|_\downarrow |S|_\uparrow$ we find

$$\frac{\nabla^2 \psi_T}{\psi_T} = \frac{\nabla^2 |S|_\downarrow}{|S|_\downarrow} + \frac{\nabla^2 |S|_\uparrow}{|S|_\uparrow} + \frac{\nabla^2 J}{J} + 2\left(\frac{\nabla |S|_\downarrow}{|S|_\downarrow} + \frac{\nabla |S|_\uparrow}{|S|_\uparrow}\right)\cdot\frac{\nabla J}{J},$$

noting that there is no cross-term between the determinants as they depend on different coordinates. By the same arguments as above we find

$$\frac{1}{|S|}\frac{\partial^2 |S|}{\partial z_i^2} = \sum_j \frac{\partial^2 s_{ij}}{\partial z_i^2} s_{ji}^{-1},$$

which means that

$$\begin{aligned}
\frac{\nabla^2\psi_s}{\psi_s} &= \sum_{ij}(\nabla^2 s^{\downarrow}_{ij})s^{\downarrow,-1}_{ji} + (\nabla^2 s^{\uparrow}_{ij})s^{\uparrow,-1}_{ji} \\
&= \sum_{ij}^{N/2}(\nabla^2\psi_{\downarrow,j}(\boldsymbol{r}_i))s^{\downarrow,-1}_{ji} + (\nabla^2\psi_{\uparrow,j}(\boldsymbol{r}_i))s^{\uparrow,-1}_{ji} \\
&= \sum_{ij}^{N/2}(\alpha^2\omega^2 r_i^2 - 2\alpha\omega(n_{x,j}+n_{y,j}+1))\psi_j(\boldsymbol{r_i})s^{\downarrow,-1}_{ji} + (\alpha^2\omega^2 r^2_{i+N/2} - 2\alpha\omega(n_{x,j}+n_{y,j}+1))\psi_j(\boldsymbol{r_{i+N/2}})s^{\uparrow,-1}_{ji} \\
&= \sum_{ij}^{N/2}(\alpha^2\omega^2 r_i^2 - 2\alpha\omega(n_{x,j}+n_{y,j}+1))s^{\downarrow}_{ij}s^{\downarrow,-1}_{ji} + (\alpha^2\omega^2 r^2_{i+N/2} - 2\alpha\omega(n_{x,j}+n_{y,j}+1))s^{\uparrow}_{ij}s^{\uparrow,-1}_{ji} \\
&= \sum_{i=1}^{N}\alpha^2\omega^2 r_i^2 - 4\alpha\omega\sum_{j}^{N/2}(n_{x,j}+n_{y,j}+1),
\end{aligned}$$

where I have used that $\sum_j s_{ij}s^{-1}_{ji} = \sum_i s^{-1}_{ji}s_{ij} = 1$. For the jastrow part

$$\frac{1}{J}\frac{\partial^2 J}{\partial z_i^2} = \sum_{j\neq i}\frac{\partial^2 f_{ij}}{\partial z_i^2} + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial z_i}\right)^2,$$

with $f_{ij} = a_{ij}r_{ij}/(1+\beta r_{ij})$, so

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

and

$$\frac{\nabla_i^2 J}{J} = \sum_{j\neq i}\frac{a_{ij}}{(1+\beta r_{ij})^2}\left[\frac{1}{r_{ij}} - \frac{2\beta}{(1+\beta r_{ij})}\right] + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial x_i}\right)^2 + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial y_i}\right)^2,$$

and finally

$$\frac{\nabla^2 J}{J} = 2\sum_{j<i}\frac{a_{ij}}{(1+\beta r_{ij})^2}\left[\frac{1}{r_{ij}} - \frac{2\beta}{(1+\beta r_{ij})}\right] + \sum_i\left[\left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial x_i}\right)^2 + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial y_i}\right)^2\right],$$

The cross terms become

$$2\left(\frac{\nabla|S|_{\downarrow}}{|S|_{\downarrow}} + \frac{\nabla|S|_{\uparrow}}{|S|_{\uparrow}}\right)\cdot\frac{\nabla J}{J} = 2\sum_i\left(\frac{1}{|s|}\frac{\partial|s|}{\partial x_i}\frac{1}{J}\frac{\partial J}{\partial x_i} + \frac{1}{|s|}\frac{\partial|s|}{\partial y_i}\frac{1}{J}\frac{\partial J}{\partial y_i}\right).$$

C.3 Derivative w.r.t α and β

The many particle generalizations of the formulas from section B.3. For α we again need the derivative of a determinant, but the arguments for the adjugate C^T being independent of the diffentiation variable used above is no longer valid. Luckily Jacobis formula says that we may still use a similar expression:

$$\frac{1}{|A|}\frac{\mathrm{d}|A|}{\mathrm{d}\alpha} = \sum_{i,j}\frac{\mathrm{d}A_{ij}}{\mathrm{d}\alpha}A^{-1}_{ji}.$$

In our case we then have

$$\frac{1}{\psi_T}\frac{\partial\psi_T}{\partial\alpha} = \sum_{i,j}\frac{\partial\psi_i(\boldsymbol{r}_j)}{\partial\alpha}s^{\downarrow,-1}_{ji} + \frac{\partial\psi_i(\boldsymbol{r}_{j+N/2})}{\partial\alpha}s^{\uparrow,-1}_{ji}.$$

$$
\begin{aligned}
\frac{\partial \psi_i(\boldsymbol{r})}{\partial \alpha} &= \omega \frac{\partial \psi_i(\boldsymbol{r})}{\partial \alpha \omega} \\
&= \omega \left(\frac{\partial \sqrt{\alpha\omega} x}{\partial \alpha} H'_{n_x}(\sqrt{\alpha\omega}x) H_{n_y}(\sqrt{\alpha\omega}y) + \frac{\partial \sqrt{\alpha\omega} y}{\partial \alpha} H_{n_x}(\sqrt{\alpha\omega}x) H'_{n_y}(\sqrt{\alpha\omega}y) \right. \\
&\qquad \left. -\frac{1}{2}(x^2+y^2) H_{n_x}(\sqrt{\alpha\omega}x) H_{n_y}(\sqrt{\alpha\omega}y) \right) e^{-\alpha\omega(x^2+y^2)/2} \\
&= \omega \left(\frac{x n_x}{\sqrt{\alpha\omega}} H_{n_x-1}(\sqrt{\alpha\omega}x) H_{n_y}(\sqrt{\alpha\omega}y) + \frac{y n_y}{\sqrt{\alpha\omega}} H_{n_x}(\sqrt{\alpha\omega}x) H_{n_y-1}(\sqrt{\alpha\omega}y) \right. \\
&\qquad \left. -\frac{1}{2}(x^2+y^2) H_{n_x}(\sqrt{\alpha\omega}x) H_{n_y}(\sqrt{\alpha\omega}y) \right) e^{-\alpha\omega(x^2+y^2)/2}.
\end{aligned}
$$

The β derivative is a lot simpler:

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

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