FYS4411 - Computational Physics II: Quantum Mechanical Systems

Project 2 - Variatonal Monte Carlo Studies of Electronic Systems.

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https://www.github.com/Oo1Insane1oO/FYS4411

June 12, 2017

Abstract

I INTRODUCTION

Using the Variational Monte Carlo, this project aims to find and analyze quantities such as the ground state energy and single-particle densities of quantum dots for so-called closed shell systems.

We use the usual approach by estimating expectation value of the ground state energy with the variational principle and minimizing. The algorithm used for the Monte Carlo method is the well known Metropolis algorithm.

The reason for using a Monte Carlo method for minimizing the trial ground state energy is because the expectation value would in general be a multi-dimensional integral depending on the number of particles and number of parameters involved in the total wave function. Such an integral is not adequately solved by traditional methods(i.e Gaussian-quadrature).

The desired result is that the Metropolis algorithm with importance sampling yields a better result both from a computational point of view. That is it finds a good estimate for the ground state energy efficiently without wasting to much time on the configuration space. The wave function only has small values in this large space meaning a homogeneous distribution of calculation points would yield a poor result, a non-homogeneous approach(such as with the Metropolis algorithm) would then, hopefully, gives a better result.

II THEORY

This section will explain the various theoretical approaches used in the project. All formulas, analytic expressions and derivations are given here. All the computational optimizations used are also given(see section II.L).

II.A HERMITE POLYNOMIALS

Hermite polynomials $H(x)$ are solutions to the differential equation

$$\frac{\mathrm{d}^2H}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}H}{\mathrm{d}x} + (\lambda - 1)H = 0 \tag{1}$$

The polynomials fulfill the orthogonality relation

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} H_n^2 \mathrm{d}x = 2^n n! \sqrt{\pi} \tag{2}$$

with the recurrence relation

$$H_{n+1} = 2xH_n - 2nH_{n-1} \tag{3}$$

and standardized relation

$$H_n = (-1)^n \mathrm{e}^{x^2} \frac{\partial^n}{\partial x^n} \mathrm{e}^{-x^2} \tag{4}$$

From equation 4 one can find an expression for the derivative of the Hermite polynomial as

$$\frac{\partial^m H_n}{\partial x^m} = 2^m m! \frac{n!}{(n-m)!} H_{n-m} \tag{5}$$

II.B HARMONIC OSCILLATOR

II.B.1 Cartesian Coordinates

The harmonic oscillator system in 2 dimensions and in natural units is given by the following Hamiltonian

$$\hat{H_0} = \frac{1}{2}\sum_{i=1}^{N}\left(-\nabla_i^2 + \omega^2 r_i^2\right) \tag{6}$$

The wave functions in this case is then:

$$\phi_{n_x,n_y}(x,y) = AH_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y)\exp\left(-\frac{\omega}{2}(x^2+y^2)\right) \tag{7}$$

where H_n is a Hermite polynomial of order n and A is a normalization constant. The quantum numbers n_x and n_y go as $n_x, n_y = 0, 1, 2\ldots$. While ω is the oscillator frequency.
The energies is

$$E = \hbar\omega\left(n_x + n_y + 1\right) \tag{8}$$

II.C FOURIER TRANSFORMATION

Given an integrable function $f : \mathbb{R} \to \mathbb{C}$ the Fourier transform to variable x is defined to be

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \mathrm{e}^{ixs} \mathrm{d}x \tag{9}$$

with $x, s \in \mathbb{R}$.
The inverse transformation is given as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{-isx} \mathrm{d}s \tag{10}$$

II.D GRADIENT DESCENT

The method of gradient descent aims to minimize a function f with respect to its n parameters $\alpha_1, \ldots, \alpha_n$. The idea is to blindly follow a portion of the gradient of the function giving the following estimate for the minimum

$$\begin{pmatrix} \alpha_1^{\text{new}} \\ \vdots \\ \alpha_n^{\text{new}} \end{pmatrix} = \begin{pmatrix} \alpha_1^{\text{old}} \\ \vdots \\ \alpha_n^{\text{old}} \end{pmatrix} - \gamma \begin{pmatrix} \frac{\partial f}{\partial x_1^{\text{old}}} \\ \vdots \\ \frac{\partial f}{\partial x_n^{\text{old}}} \end{pmatrix} \tag{11}$$

with γ being the step-size determining the how much(portion) of the gradient to follow.

II.E CONJUGATE GRADIENT METHOD

Suppose we have a linear system defined as

$$A\vec{x} = \vec{b} \tag{12}$$

where A is a nxn real, symmetric and positive definite matrix while $\vec{x}$ and $\vec{b}$ are a non-zero real vectors.
Define now the conjugate directions of two vectors $\vec{x}_i, \vec{x}_j : \mathbb{R} \to \mathbb{R}$ giving the constraint

$$\vec{x}_i^T A \vec{x}_j = \vec{0} \tag{13}$$

This means that in the iterative process of finding $\vec{x}$ we perform searches within the conjugate directions of $\vec{x}$.
Since the conjugate constraint(equation 13) is defined by an inner product within the space A is defined, the two vectors $\vec{x}_i$ and $\vec{x}_j$ are orthogonal. If we now define a span P

$$P = \{\vec{p}_1, \ldots, \vec{p}_n\} \tag{14}$$

consisting of n mutually orthogonal conjugate directions $\vec{p}_i$, we have a basis for $\mathbb{R}^n$. Expanding the solution x_{i+1} to equation 12 in the mentioned basis

$$\vec{x} = \sum_{i=1}^{n} C_i \vec{p}_i \tag{15}$$

the linear system can be rewritten as

$$A\vec{x} = \sum_{i=1}^{n} C_i A \vec{p}_i = \vec{b} \tag{16}$$

Giving the inner product

$$\vec{p}_k^T A \vec{x} = \sum_{i=1}^{n} C_i \vec{p}_k^T A \vec{p}_i \tag{17}$$

and we can define the coefficients C_k as

$$C_k = \frac{\vec{p}_k^T \vec{b}}{\vec{p}_k^T A \vec{p}_k} \tag{18}$$

The problem at hand is then to choose a sequence of n conjugate directions P and compute the coefficients C_k.

II.E.1 Iterative Method

The conjugate gradient method can in a similar manner be used on an iterative basis. We start with an initial guess $\vec{x}_0$ for the solutions and consider the linear system

$$A\vec{x} = \vec{b} - \vec{r} \tag{19}$$

where $A, \vec{x}$ and $\vec{b}$ are defined as before and $\vec{r}$ is a so-called residual.
Let $\vec{r}_k$ be the residual at the k-th step with a negative gradient. Using a similar approach as before we get that the conjugate direction $\vec{p}_{i+1}$ is

$$\vec{p}_{i+1} = \vec{r}_k - \frac{\vec{p}_k^T A\vec{r}_k}{\vec{p}_k^T A\vec{p}_k}\vec{p}_k \tag{20}$$

The iterative process is then to compute the directions and then solve the arising linear system by computing the coefficients as given in equation 18.
The iterative process is then to compute

$$\vec{x}_{k+1} = \vec{x}_k + C_k\vec{p}_{k+1} \tag{21}$$

with

$$C_k = \frac{\vec{p}_k^T\vec{r}_k}{\vec{p}_k^T A\vec{p}_k} \tag{22}$$

The residual $\vec{r}_k$ at the k-th step is defined from equation 19 as

$$\vec{r}_k = \vec{b} - A\vec{x}_k \tag{23}$$

II.F LAPLACE EXPANSION

Given a $n \times n$ matrix $M = [m_{ij}]$ and $i, j \in [1, \ldots, n]$, then the determinant of M is

$$\det(M) = \sum_{j=1}^{n} m_{ij} C_{ij} \tag{24}$$

where C_{ij} is the i, j-element of the so-called cofactor matrix defined as the sub-matrix arising from removing the i-th row and j-th column from M. The cofactor matrix element is given as

$$C_{ij} = (-1)^{i+j} M_{ij} \tag{25}$$

where the indices i and j run from 1 up to $n-1$ [9].

II.G DERIVATIVE OF DETERMINANT

We can express the derivative with respect to t for a square matrix $A(t)$ of size n which has a differentiable map $\mathrm{d}A \in \mathbb{R} \to \mathbb{R}^n$ as

$$\frac{\partial A(t)}{\partial t} = \mathrm{Tr}\left(\mathrm{adj}\,(A(t))\,\frac{\partial A(t)}{\partial t}\right) \tag{26}$$

where Tr is the trace and adj is the adjugate(transpose of cofactor matrix). This relation is known as Jacobi's formula [9].
We can specialize Jacobi's formula to

$$\frac{\partial A(t)}{\partial t} = \det(A)\,\mathrm{Tr}\left(A(t)^{-1}\frac{\partial A(t)}{\partial t}\right) \tag{27}$$

if A is invertible. This relation follows from the definition of the adjugate which gives

$$A\mathrm{adj}\,(A) = \det(A)\mathbb{1} \tag{28}$$

and in turn if A is invertible

$$A^{-1} = \frac{1}{\det(A)}\mathrm{adj}\,(A) \tag{29}$$

(known as Cramers' rule). Here $\mathbb{1}$ is the $n \times n$ identity matrix.

II.H METROPOLIS-HASTINGS ALGORITHM

The Metropolis algorithm bases itself on moves (also called transitions) as given in a Markov process(or Markov chain). Define a probability distribution function(PDF) $w_j(t)$ with a transition probability $w(i \to j)$ which for a given time-step yields in the Markov formula

$$w_i(t+\varepsilon) = \sum_j w(j \to i)\, w_j(t) \tag{30}$$

The transition probability is defined with an acceptance probability distribution $A(j \to i)$ and a proposed probability distribution $T(j \to i)$ as

$$w(j \to i) = A(j \to i)\, T(j \to i) \tag{31}$$

The acceptance A is the probability for the move to be accepted and the proposal T is different for each problem.
In order for this transition chain to reach a desired convergence and reversibility we have the well known condition for detailed balance[11]. This condition gives us that the probability distribution functions satisfy the following condition

$$w_i T_{i\to j} A_{i\to j} = w_j T_{j\to i} A_{j\to i} \Rightarrow \frac{w_i}{w_j} = \frac{T_{j\to i} A_{j\to i}}{T_{i\to j} A_{i\to j}} \tag{32}$$

We now need to choose an acceptance which fulfills equation 32 and a common choice is the Metropolis condition

$$A_{j\to i} = \min\left(1, \frac{w_i T_{i\to j}}{w_j T_{j\to i}}\right) \tag{33}$$

The Metropolis-Hastings algorithm is thus

(i) Pick initial state i at random.

(ii) Pick proposed state at random in accordance to $T_{j\to i}$.

(iii) Accept state according to $A_{j\to i}$.

(iv) Jump to step (ii) until a specified number of states have been generated.

(v) Save the state i and jump to step (ii).

II.I VARIATIONAL PRINCIPLE

The variational principle states the following restriction on the ground state energy for a given symmetry

$$E_0 \leq \langle E[\Phi_T] \rangle = \int \phi_T^* \hat{H} \phi_T \, \mathrm{d}\tau = \langle \phi_T | \hat{H} | \phi_T \rangle \tag{34}$$

that is the ground state energy E_0 is bounded by the expectation value of the trial energy.

II.J IMPORTANCE SAMPLING

In order to use the Metropolis algorithm as explained in section II.H, we need to find the proposal probability distribution labeled $T_{j\to i}$. This is what is known as importance sampling.
This section will derive the importance sampling by using the Fokker-Planck equation for one particle

$$\frac{\partial P}{\partial t} = D \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} - F\right) P(x,t) \tag{35}$$

where F is a drift term and D is a diffusion constant, and the Langevin equation

$$\frac{\partial x(t)}{\partial t} = DF(x(t)) + \eta \tag{36}$$

where η is a Gaussian distributed random variable.

II.J.1 Quantum Force

We will in this section give an outline of the derivation for the quantum force. See [3] for more.
Since we are working with a isotropic diffusion characterized by a time-dependant probability density our system must obey the summed total Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \sum_i D \frac{\partial}{\partial x_i}\left(\frac{\partial}{\partial x_i} - F_i\right) P(x,t) \tag{37}$$

where F_i is now the i'th component of the drift velocity term(given by an external potential). Since the probability is assumed to be convergent, that is it converges to a stationary probability density the time dependence at this point is zero for all i. We also know that the drift should be of form $F = g(x)\frac{\partial P}{\partial x}$ giving

$$\frac{\partial^2 P}{\partial {x_i}^2} = P\frac{\partial g}{\partial P}\left(\frac{\partial P}{\partial x_i}\right)^2 + Pg\frac{\partial^2 P}{\partial {x_i}^2} + g\left(\frac{\partial P}{\partial x_i}\right)^2 \tag{38}$$

Now we may use the condition for stationary density meaning the left hand side of equation 38 must equal zero giving that $g = 1/P$(only possibility the derivatives cancel). Inserting in $P = \psi_T$ we get that the expression for the quantum force is

$$F_i = \frac{2}{\Psi_T}\nabla_i \Psi_T \tag{39}$$

Notice that the quantum force is defined individually for each particle because of the assumption of of stationary probability density.

II.J.2 Solution

Using Eulers method(Euler-Maruyama method[10]) on the Langevin equation(equation 36) one obtains the new positions

$$y = x + DF(x)\Delta t + \xi\sqrt{\Delta t} \tag{40}$$

with $D = 1/2$ in natural units due to the kinetic energy term and Δt is a time-step parameter. The random variable ξ is within a Gaussian distribution of variance one and standard deviation zero.
For the differential equation (equation 35) we insert in for the quantum force given in equation 39 and arrive at the following diffusion equation

$$\frac{\partial P}{\partial t} = -D\frac{\partial^2 P}{\partial r^2} \tag{41}$$

This equation is solved by using a Fourier transform in the spatial coordinate r according to equation 9 giving the equation

$$\frac{\partial \tilde{P}(s,t)}{\partial t} = -Ds^2\tilde{P}(s,t) \tag{42}$$

with solution

$$\tilde{P}(s,\Delta t) = \tilde{P}(s,0)\mathrm{e}^{-Ds^2\Delta t} \tag{43}$$

Initially the probability density is centered at $D\Delta t F(x)$, that is the drift term. This can be expressed terms of a Dirac-delta function, meaning

$$P(y,x,0) = \delta(y - D\Delta t F(x)) \tag{44}$$

where y is given in equation 40. Making an inverse transformation as described in equation 10 and solving the subsequent transcendental integral yields in

$$P(y,x,\Delta t) = \frac{1}{\sqrt{4\pi D\Delta t}}\exp\left(-\frac{(y-x-D\Delta t F(x))^2}{4D\Delta t}\right) \tag{45}$$

which gives us the acceptance

$$A_{y\to x} = \min\left(1, \frac{|\psi_T(y)|^2 P(y,x,\Delta t)}{|\psi_T(x)|^2 P(x,y,\Delta t)}\right) \tag{46}$$

II.K VMC

This section will explain and derive the equations involved in the Variational Monte Carlo method[3].
The whole section will assume that we have the following trial wave function, ψ_T

$$\psi_T(\vec{r}_1,\ldots,\vec{r}_N) \equiv \det(\phi_1(\vec{r}_1,\alpha),\ldots,\phi(\vec{r}_N,\alpha))\prod_{i<j}^{N}\exp\left(\frac{a r_{ij}}{1+\beta r_{ij}}\right) \tag{47}$$

with the $\vec{r}$'s being the position of the electrons and the ϕ's being the wave function to some known system(i.e harmonic oscillator). The position r_{ij} is a relative distance $\left|\vec{r}_i - \vec{r}_j\right|$ while α and β are variational parameters and a is a specific constant dependant of the total spin symmetry of electron i and j as

$$a = \begin{cases} 1, & \text{anti-parallel spin} \\ \dfrac{1}{3}, & \text{parallel spin} \end{cases} \tag{48}$$

This is also known as a Pade-Jastrow factor.
We also define the total Hamiltonian of the system for the quantum dot case as

$$\hat{H} = \hat{H}_O + \hat{H}_I \tag{49}$$

with $\hat{H}_O$ being the harmonic oscillator defined in equation 6 and $\hat{H}_I$ being the Hamiltonian for the electron interactions(Coulomb interaction) defined as

$$\hat{H}_I = \sum_{i<j} \frac{1}{r_{ij}} \tag{50}$$

Lastly, we work in natural units setting $\hbar = c = 1$, and all the above equations(equations 47, 48, 49 and 50) also assume natural units.

II.K.1 Expectation Value and Local Energy

Given the Hamiltonian equation 49 and a trial wave function $\Psi_T(R, \Lambda)$ and using the variational principle, as given in equation 34 the upper bound for the ground state energy E_0 if $H(r)$ is

$$E[\hat{H}(R,\Lambda)] \leq \left\langle \hat{H} \right\rangle = \frac{\langle \Psi_T | \hat{H} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \tag{51}$$

where $R = (r_1, \ldots, r_N)$ is the positions to N particles and $\Lambda = (\lambda, \ldots, \lambda_M)$ are the M variational parameters.
Now we can expand the trial wave function $\Psi_T(R, \Lambda)$ in the orthonormal eigenstates of the Hamiltonian $\hat{H}$(which form a complete set)

$$\Psi_T(r) = \sum_i c_i \Psi_i(r) \tag{52}$$

and the upper bound given in equation 51 is

$$E_0 \leq \frac{\sum_{ij} c_i c_j^* \left\langle \Psi_j \right| \hat{H} \left| \Psi_i \right\rangle}{\sum_{ij} c_i c_j^* \left\langle \Psi_j \middle| \Psi_i \right\rangle} = \frac{\sum_n a_n^2 E_n}{\sum_n a_n^2} \tag{53}$$

where the eigenequation for the Hamiltonian $\hat{H}\Psi_n = E_n \Psi_n$ was used. The expression given in equation 51 is the expectation value we evaluate in each variational step that is we choose α according to some minimization algorithm and re-evaluate the expectation value.
In order to introduce the transition probability as given in the Metropolis algorithm(see section II.H) the expectation value, equation 53, needs to be rewritten in terms of a PDF. We can define this as

$$P(R) \equiv \frac{|\Psi_T(R)|^2}{\int |\Psi_T(R)|^2 \mathrm{d}R} \tag{54}$$

Now we observe that if we define a quantity

$$E_L(R,\Lambda) \equiv \frac{1}{\Psi_T(R,\Lambda)} \hat{H} \Psi_T(R,\Lambda) \tag{55}$$

which is the so-called local energy. The expectation value given in equation 53 can be rewritten as

$$E[H] = \int P(R) E_L(R,\Lambda) \mathrm{d}R \approx \frac{1}{N} \sum_{i=1}^{N} P(r_i,\Lambda) E_L(r_i,\Lambda) \tag{56}$$

which is of the form given in equation 30 and N is the number of states(or Monte Carlo cycles).

II.L Optimization

In the method described in section II.K the heavy load in terms of calculation lies within the calculation of the determinant ratio given in equations 46 and 39. This section will derive an expression for these ratios in terms of computation time. We will in the whole section assume we only move one particle at a time in the Monte Carlo cycle.

II.L.1 Determinant Ratio

In the Metropolis algorithm we calculate a ratio of determinants in the Metropolis test. Starting by defining a Slater determinant Matrix D with entries defined as

$$D_{ij} \equiv \phi_j(r_i) \tag{57}$$

where the ϕ's are defined as in section II.K.
In terms of cofactors C_{ij} we have

$$\det(D) = \sum_{j=1}^{N} D_{ij} C_{ij} \tag{58}$$

If we now take into light the mentioned assumption about moving only one particle at a time the determinant given in equation 57 only gets a change of one row.
Defining the ratio as

$$R \equiv \frac{\det(D(x^{\text{new}}))}{\det(D(x^{\text{old}}))} \tag{59}$$

Using the fact that when moving the particle at position r_i the cofactors remain unchanged ($C^{\text{new}} = C^{\text{old}}$) and inserting in equation 58 into equation 59 we have

$$R = \frac{\sum_{j=1}^{N} D_{ij}(r^{\text{new}}) C_{ij}(r^{\text{old}})}{\sum_{j=1}^{N} D_{ij}(r^{\text{old}}) C_{ij}(r^{\text{old}})} \tag{60}$$

Since the Slater is square(closed shell) and invertible(since the determinant is non-zero[9]), we have the following ratio

$$D^{-1}_{ji} = \frac{C_{ij}}{\det(D)} \tag{61}$$

inserting this into equation 60 we get

$$R = \frac{\sum_{j=1}^{N} D_{ij}(r^{\text{new}}) D^{-1}_{ji}(r^{\text{old}}) |D|}{\sum_{j=1}^{N} D_{ij}(r^{\text{old}}) D^{-1}_{ji}(r^{\text{old}}) |D|} \tag{62}$$

We also have

$$\sum_{k=1}^{N} D_{ik} D^{-1}_{kj} = \delta_{ij} \tag{63}$$

from the definition of the inverse, meaning the denominator in equation 62 is equal to 1 and the ratio is finally(with equation 57 inserted)

$$R = \sum_{j=1}^{N} \phi_j(r_i^{\text{new}}) \phi^{-1}_{ji}(r^{\text{old}}) \tag{64}$$

We can follow a similar approach to find the ratio given in equation 39 for the quantum force. The expression is simply

$$\frac{\nabla_i |D(r_i)|}{|D(r_i)|} = \sum_{j=1}^{N} \nabla_i \phi_j(r_i) \phi^{-1}_{ji}(r) \tag{65}$$

And a similarly for the Laplacian

$$\frac{\nabla_i^2 |D(r_i)|}{|D(r_i)|} = \sum_{j=1}^{N} \nabla_i^2 \phi_j(r_i) \phi^{-1}_{ji}(r) \tag{66}$$

The only difference is that rather then looking at new and old positions we look at the change in the respective row as the derivative.

II.L.2 Inverse of Matrix

In section II.L.1 we derived a formula for calculating the ratio of determinants by the inverse of the old determinant when only one row is changed. This section gives a formula for updating the inverse of a matrix in that case. The formula is

$$D^{-1}_{kj}(r^{\text{new}}) = \begin{cases} D^{-1}_{kj}(r^{\text{old}}) - \dfrac{D^{-1}_{ik}(r^{\text{old}})}{R} \displaystyle\sum_{l=1}^{N} D_{il}(r^{\text{new}}) D^{-1}_{lj}(r^{\text{old}}), & j \neq i \\ \dfrac{D^{-1}_{ik}(r^{\text{old}})}{R} \displaystyle\sum_{l=1}^{N} D_{il}(r^{\text{old}}) D^{-1}_{lj}(r^{\text{old}}), & j = i \end{cases} \tag{67}$$

as described by Sherman and Morris [3, 8]. The factor R is just the determinant ratio as described in equation 64.

II.L.3 Derivative Ratios

In the calculation of the local energy and quantum force we need to calculate the ratio between the derivatives of the trial wave function and the wave function it self. In this section we will derive a formula for these ratios based on the mentioned fact that we move only one particle at a time.
We start with the first derivative and define the one body part to be ψ_ϕ and the correlation term(Jastrow) to be ψ_J meaning $\psi_T = \psi_\phi \psi_J$. This gives the ratio

$$\frac{\nabla\psi_T}{\psi_T} = \frac{\nabla\psi_\phi}{\psi_\phi} + \frac{\nabla\psi_J}{\psi_J} \tag{68}$$

and for the second derivative we have

$$\frac{\nabla^2\psi_T}{\psi_T} = \frac{\nabla^2\psi_\phi}{\psi_\phi} + \frac{\nabla^2\psi_J}{\psi_J} + 2\frac{\nabla\psi_\phi}{\psi_\phi}\cdot\frac{\nabla\psi_J}{\psi_J} \tag{69}$$

For one-body part ψ_ϕ we know that the expression is just a determinant(from equation 47). Using equations 65 and 66 the expressions for the derivative ratios is

$$\begin{aligned}\frac{\nabla\psi_\phi}{\psi_\phi} &= \sum_{j=1}^{N}\nabla_i\phi_j(r_i)\psi^{-1}_{\phi,ji}(\vec{r})\\ \frac{\nabla^2\psi_T}{\psi_T} &= \sum_{j=1}^{N}\nabla_i^2\phi_j(r_i)\psi^{-1}_{\phi,ji}(\vec{r})\end{aligned} \tag{70}$$

For the correlation factor ψ_J we have an exponential form(see equation 47). The first derivative ratio is thus

$$\left[\frac{\nabla\psi_J}{\psi_J}\right]_x = \sum_{i=1}^{k-1}\frac{x_i - x_k}{r_{ik}}\frac{\partial f_{ik}}{\partial r_{ik}} - \sum_{i=k+1}^{N}\frac{x_k - x_i}{r_{ki}}\frac{\partial f_{ki}}{\partial r_{ki}} \tag{71}$$

due to the fact that the Jastrow-factor factor g is only dependant of the relative distance r_{ij} and is of exponential form and only the $N-1$ terms differentiated survive.
For the second derivative ratio we have similarly

$$\left[\frac{\nabla^2\psi_J}{\psi_J}\right]_x = \sum_{i,j\neq k}\frac{(\vec{r}_k - \vec{r}_i)(\vec{r}_k - \vec{r}_j)}{r_{ki}r_{kj}}\frac{\partial f_{ki}}{\partial r_{ki}}\frac{\partial f_{kj}}{\partial r_{kj}} + \sum_{j\neq k}\left(\frac{\partial^2 f_{kj}}{\partial {r_{kj}}^2} + \frac{2}{r_{kj}}\frac{\partial f_{kj}}{\partial r_{kj}}\right) \tag{72}$$

The factor f_{ij} is just the function appearing in the exponent of the Jastrow factor.
See [3] for full derivation.

II.M STATISTICAL ANALYSIS

Since Monte Carlo simulations can be considered to be computer experiments the resulting data can be analysed with the same statistical theory as one would with experimental data. This section will give a brief overview of some of the statistical concepts and explain the method of Blocking(for estimating the standard deviation).

II.M.1 STANDARD DEVIATION, VARIANCE AND COVARIANCE

Given a PDF $P(x)$ the mean value, variance and covariance is

$$\bar{x}_n \equiv \frac{1}{n}\sum_{k=1}^{n}x_k \tag{73}$$

$$\mathrm{var}(x) \equiv \frac{1}{n}\sum_{k=1}^{n}(x_k - \bar{x}_n)^2 \tag{74}$$

$$\mathrm{cov}(x) \equiv \frac{1}{n}\sum_{kl}(x_k - \bar{x}_n)(x_l - \bar{x}_n) \tag{75}$$

for a finite size sample.

II.M.2 Central Limit Theorem

The central limit theorem states that given a PDF P_{X_n} for a sample X_n the mean value can be expressed as

$$\lim_{n\to\infty} p_{\bar{X}_n}(x) = \sqrt{\frac{n}{2\pi\sigma(X)^2}}\exp\left(-\frac{n(x-\bar{X}_n)^2}{2\sigma(X)^2}\right) \tag{76}$$

where $\sigma^2(X)$ is the variance of the sample.

II.M.3 Statistical Error

The error in a sample is just the spread of the mean, i.e the variance of said sample. Set a finite size sample X_n the error would be

$$\sigma_X^2 = \mathrm{var}\left(\bar{X}_n\right) = \frac{1}{n^2}\sum_{ij}\mathrm{cov}\left(X_i, X_j\right) \tag{77}$$

Using the central limit theorem we can approximate the real mean as

$$\langle x_i\rangle \approx \frac{1}{n}\sum_{k=1}^{n} x_k = \bar{x} \tag{78}$$

which gives the approximative covariance

$$\mathrm{cov}\left(X_i, X_j\right) \approx \left\langle (x_i-\bar{x})(x_j-\bar{x})\right\rangle = \frac{1}{n}\mathrm{cov}(x) \tag{79}$$

and the error is thus

$$\sigma_X^2 = \frac{1}{n}\mathrm{cov}(x) \tag{80}$$

We can split this equation in part giving

$$\begin{aligned}\sigma_X^2 &= \frac{1}{n}\mathrm{var}(x) + \frac{1}{n}\left(\mathrm{cov}(x) - \mathrm{var}(x)\right)\\ &= \frac{1}{n^2}\sum_{k=1}^{n}(x_k-\bar{x}_n) + \frac{2}{n^2}\sum_{k<l}(x_k-\bar{x}_n)(x_l-\bar{x}_n)\end{aligned} \tag{81}$$

II.M.4 Autocorrelation Function

Writing the second term in our error given in equation 81 (the so-called correlation term) as a partial sums gives

$$f_d = \frac{1}{n-d}\sum_{k=1}^{n-d}(x_k-\bar{x}_n)(x_{k+d}-\bar{x}_n) \tag{82}$$

which this we can define the autocorrelation function k_d as

$$k_d \equiv \frac{f_d}{\mathrm{var}(x)} \tag{83}$$

The sample error is now

$$\sigma^2 = \frac{\tau}{n}\mathrm{var}(x) \tag{84}$$

with τ defined as the autocorrelation time

$$\tau \equiv 1 + 2\sum_{d=1}^{n-1} k_d \tag{85}$$

II.M.5 Blocking

The method of blocking estimates the standard deviation. We start by first defining a sample quantity χ of n samples and assume that the standard deviation of the mean of χ is given by

$$\sigma_\chi = \sqrt{\frac{1}{n}\left(\langle\chi^2\rangle - \langle\chi\rangle^2\right)} \tag{86}$$

Obviously this is wrong if χ is a set of correlated samples. However, we can rewrite equation 86 with equation 85 giving

$$\sigma_\chi = \sqrt{\frac{1+\frac{2\tau}{\Delta t}}{n}\left(\langle\chi^2\rangle - \langle\chi\rangle^2\right)} \tag{87}$$

where Δt is the time between each sample.
If we have that $\Delta t \gg \tau$ then the assumption for non-correlation still hold, if this is not the case we may use the method of blocking. The method is to basically divide the sample sequence into blocks of size τ(meaning sample j of block i is uncorrelated to sample j of block $i+1$). The total mean and variance is then obtained by calculating the mean of blocks $\chi_i, \ldots, \chi_{n_{\text{blocks}}}$.
The second problem is to find τ. This is solved by making a plot of the standard deviation and divide the blocks accordingly. The standard deviation will increase and reach a convergence as the block size increases.

III SETUP

See https://www.github.com/Oo1Insane1oO/FYS4411 for C++ program for the VMC calculations.
The program sets up the basis in Cartesian coordinates(class Basis in basis.cpp) and sets up the wave function before running the calculations.
All stand alone methods are given in class Methods(methods.cpp) and the VMC part is done in class VMC.
The main file sets up the class objects and takes care of dividing the problem for MPI(and runs with MPI). The variational parameters are gathered to root process in the end and averaged. All the processes write to their own respective files.
The repository also contains a python script file for the blocking analysis(readBinary.py).
The function which runs the VMC calculations splits the wave function in two, one for spin up states and one for spin down and uses the different optimizations mentioned in section II.L(functions themselves are given in methods.cpp).
After the Metropolis sampling is done, we use the Steepest descent method for minimization.
The whole sampling is run one last time with the optimal parameters and results are dumped to binary files(one for each process).

IV RESULTS

Table of Results

N	ω	$\langle E\rangle$	σ^2	$\langle V\rangle$	$\langle K\rangle$	α	β
2	1.0	2.95831	5.07406e-10	1.79365	-1.16466	0.91509	0.33318
	0.5	1.66193	2.39178e-10	1.05746	-0.60447	0.91506	0.33313
	0.1	0.48838	1.20155e-10	0.36194	-0.12644	0.91506	0.33309
	0.05	0.31837	1.32613e-10	0.26227	-0.0561	0.91506	0.33309
	0.01	0.13167	6.70777e-11	0.12295	-0.00872	0.91507	0.33309
6	1.0	19.9421	2.59559e-08	15.78908	-4.15301	0.91619	0.33646
	0.5	11.74103	1.09932e-08	9.68788	-2.05315	0.91545	0.33515
	0.1	3.85914	2.69821e-09	3.54323	-0.31591	0.91464	0.33197
	0.05	2.6081	1.52649e-09	2.55371	-0.05439	0.91433	0.3293
	0.01	1.44591	3.59932e-09	1.64754	0.20163	0.91435	0.32314
12	1.0	65.07053	6.15884e-07	55.66897	-9.40155	0.9369	0.43675
	0.5	39.22833	2.49011e-07	34.95471	-4.27361	0.93188	0.44864
	0.1	13.96408	1.51215e-07	14.26539	0.30132	0.91679	0.4345
	0.05	10.03819	1.65441e-07	11.12425	1.08607	0.91121	0.4146
	0.01	6.68697	2.17118e-07	8.74482	2.05786	0.91124	0.38367
20	1.0	162.22928	2.57523e-06	139.06938	-23.15991	1.02408	0.89279
	0.5	102.24884	2.19823e-06	92.62211	-9.62674	0.9802	0.90839
	0.1	42.02145	2.47687e-06	44.3903	2.36885	0.86263	0.82274
	0.05	32.81069	3.51335e-06	37.05155	4.24087	0.8525	0.75049
	0.01	25.9103	2.84533e-06	31.83161	5.92132	0.88898	0.72217

V DISCUSSION

V.A With Jastrow

V.A.1 Energies

As we can see from section IV the energies are rather strange compared to the Hartree-Fock energies. Some of the energies obtained by the VMC calculations are higher, which they should not be. There may be several reasons for this, we might not have found the optimal parameters, or(much more likely) there is an error in the code.

V.A.2 Error

With that said, the standard deviation is fairly good, however it increases with the number of particles suggesting there might be an error in how the derivatives are calculated in the VMC loop.
For the blocking part we have plots which have the expected form, but are a bit jagged. The optimal standard deviation was found by smoothing out the graph and taking an average over the most stationary area(the area with lowest gradient).

V.B Without Jastrow

As for the calculations without the Jastrow factor the energies look good. We have no ground to compare with the energies with Jastrow factor, however we expect the energies to be lower when the Jastrow factor is included.

V.C Speed-up

We see that with MPI the speed-up almost follows by a factor number of processes, suggesting we have an almost perfect speed-up ratio per number of processes.

VI CONCLUSION

We have in this project set up a program for calculating the ground-state energy of an electron system trapped in a quantum-dot with the harmonic oscillator functions as basis functions.
The resulting energies do not look promising as they are higher than the ones obtained from Hartree-Fock calculations. We conclude with that the poor results are due to an error in the code.

VII Appendix

VII.A ANALYTIC EXPRESSION FOR LOCAL ENERGY

VII.A.1 Two Electron Case

We start by finding the local energy in the case with two electrons. The trial wave function is in this case(related to equation 7) using equation 47

$$\psi_T(\vec{r}_1,\vec{r}_2) = A\exp\Big(-\frac{\alpha\omega}{2}\left(r_1^2+r_2^2\right)\Big)\exp\Big(\frac{ar_{12}}{1+\beta r_{12}}\Big) \tag{88}$$

Using the definition of the trial wave function, equation 55 and the total Hamiltonian(equation 49) the local energy with equation 55 is

$$E_L = \frac{1}{\psi_T}\left(\hat{H}_O\psi_T + \hat{H}_I\psi_T\right) \tag{89}$$

we solve the first part $\hat{H}_O\psi_T$

$$\hat{H}_O\psi_T = \frac{1}{2}\left(-\nabla_1^2 - \nabla_2^2 + \omega^2\left(r_1^2+r_2^2\right)\right)\psi_T \tag{90}$$

Starting with the Laplacian for electron 1 and solving the second derivative with respect to x_1 we have

$$\frac{\partial^2\psi_T}{\partial {x_1}^2} = A\exp\Big(-\frac{\alpha\omega}{2}\left(r_2^2+y_1^2\right)\Big)\frac{\partial^2}{\partial {x_1}^2}\left[\exp\Big(-\frac{\alpha\omega}{2}x_1^2 + \frac{a}{\beta+\frac{1}{r_{12}}}\Big)\right] \tag{91}$$

Starting with the first derivative in the exponential we get

$$\left.\begin{aligned}\frac{\partial}{\partial x_1}\left[-\frac{\alpha\omega}{2}x_1^2\right] &= -\alpha\omega x_1 \\ \frac{\partial}{\partial x_1}\left[\frac{a}{\beta+\frac{1}{r_{12}}}\right] &= \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\end{aligned}\right\} \Rightarrow \frac{\partial\psi_T}{\partial x_1} = \left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)\psi_T \tag{92}$$

meaning equation 91 is

$$\begin{aligned}\frac{\partial^2\psi_T}{\partial {x_1}^2} &= A\exp\left(-\frac{\alpha\omega}{2}\left(r_2^2+y_1^2\right)\right)\frac{\partial}{\partial x_1}\left[-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right]\exp\left(-\frac{\alpha\omega}{2}x_1^2 + \frac{a}{\beta+\frac{1}{r_{12}}}\right) \\ &= \frac{\partial}{\partial x_1}\left[\left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})}\right)\psi_T\right]\end{aligned} \tag{93}$$

Using the product rule for differentiation and starting with the first expression we get that

$$\frac{\partial}{\partial x_1}\left[-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right] = -\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3} \tag{94}$$

giving

$$\begin{aligned}\frac{\partial^2\psi_T}{\partial {x_1}^2} &= \psi_T\frac{\partial}{\partial x_1}\left[-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right] + \left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)\frac{\partial\psi_T}{\partial x_1} \\ &= \left[-\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3} + \left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)^2\right]\psi_T\end{aligned} \tag{95}$$

The second derivative with respect to y_1 yields with a similar derivation

$$\frac{\partial^2\psi_T}{\partial {y_1}^2} = \left[-\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3} + \left(-\alpha\omega y_1 + \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)^2\right]\psi_T \tag{96}$$

The second derivatives with respect to x_2 and y_2, are derived in a similar manner, only we get a change in signs when differentiating r_{12}. This gives

$$\frac{\partial^2\psi_T}{\partial {x_2}^2} = \left[-\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3} + \left(\alpha\omega x_2 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)^2\right]\psi_T \tag{97}$$

and

$$\frac{\partial^2\psi_T}{\partial {y_2}^2} = \left[-\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3} + \left(\alpha\omega y_2 + \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)^2\right]\psi_T \tag{98}$$

gathering equations 95, 96, 97 and 98 we get

$$\begin{aligned}(\nabla_1^2+\nabla_2^2)\psi_T &= \frac{\partial^2\psi_T}{\partial {x_1}^2} + \frac{\partial^2\psi_T}{\partial {y_1}^2} + \frac{\partial^2\psi_T}{\partial {x_2}^2} + \frac{\partial^2\psi_T}{\partial {y_2}^2} \\ &= \left[-4\alpha\omega + \frac{4a}{r_{12}(1+\beta r_{12})^2} - \frac{2a(1+3\beta r_{12})}{r_{12}(1+\beta r_{12})^3} + \alpha^2\omega^2\left(r_1^2+r_2^2\right) - \frac{2a\alpha\omega r_{12}}{(1+\beta r_{12})^2} + \frac{2a^2}{(1+\beta r_{12})^4}\right]\psi_T \qquad (99) \\ &= \left[\alpha^2\omega^2\left(r_1^2+r_2^2\right) - 4\alpha\omega - \frac{2a\alpha\omega r_{12}}{(1+\beta r_{12})^2} + \frac{2a}{(1+\beta r_{12})^2}\left(\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{1+\beta r_{12}}\right)\right]\psi_T \qquad (100)\end{aligned}$$

and the local energy(equation 89) is finally

$$E_L = \frac{1}{2}\omega^2\left(1-\alpha^2\right)\left(r_1^2+r_2^2\right) + 2\alpha\omega - \frac{a}{(1+\beta r_{12})^2}\left(\frac{a}{(1+\beta r_{12})^2} - \alpha\omega r_{12} + \frac{1}{r_{12}} - \frac{2\beta}{1+\beta r_{12}}\right) + \frac{1}{r_{12}} \tag{101}$$

VII.A.2 General Case

For the general case with N electrons(still closed shell) the local energy is defined as in equation 89, but with ψ_T defined as in equation 47. The Laplacian in this case would then be

$$\nabla_N^2 = \sum_{k=1}^{N}\nabla_k^2 = \sum_{k=1}^{N}\left(\frac{\partial^2}{\partial {x_k}^2} + \frac{\partial^2}{\partial {y_k}^2}\right) \tag{102}$$

that is a sum over the single-particle spacial Laplacians.
As mentioned we derive an expression based on the fact that we only move one particle at a time. This means we can rewrite the derivative ratio given in the local energy by using the formulas from section II.L. We see that we need the second derivatives to the single particle wave functions. The single particle wave function is(equation 7)

$$\Phi_{kj} = \phi_{n_{x_j} n_{y_j}}(r_k, \alpha) = H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_k\right) H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_k\right) \exp\left(-\frac{\alpha\omega}{2}\left(x_k^2 + y_k^2\right)\right) \tag{103}$$

The expression to be solved for the k-th particle is thus

$$\begin{aligned}\nabla_k^2 \Phi_{kj} = H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_k\right) \exp\left(-\frac{\alpha\omega}{2}y_k^2\right) \frac{\partial^2}{\partial {x_k}^2}\left(H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_k\right) \exp\left(-\frac{\alpha\omega}{2}x_k^2\right)\right) \\ + H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_k\right) \exp\left(-\frac{\alpha\omega}{2}x_k^2\right) \frac{\partial^2}{\partial {y_k}^2}\left(H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_k\right) \exp\left(-\frac{\alpha\omega}{2}y_k^2\right)\right)\end{aligned} \tag{104}$$

Solving the differential for x_k and similarly y_k by substituting $s = \sqrt{\alpha\omega}x_k = \sqrt{\alpha\omega}y_k$(respectively) and labeling $n_x, n_y \to n$ and defining

$$\begin{aligned} e(x_k) &\equiv \exp\left(-\frac{\alpha\omega}{2}x_k^2\right) \\ e(y_k) &\equiv \exp\left(-\frac{\alpha\omega}{2}y_k^2\right)\end{aligned} \tag{105}$$

Using the product rule for differentiation and equation 5 for the derivative of the Hermite polynomials with the recursion relation given in equation 3 for $H_n(s)$ gives

$$\begin{aligned}\alpha\omega\frac{\partial^2}{\partial s^2}\left(H_n(s)e(s)\right)\right) &= \alpha\omega\left(\frac{\partial^2 H_n}{\partial s^2} - 2s\frac{\partial H_n}{\partial s} + \left(s^2-1\right)H_n(s)\right)e(s) \\ &= \alpha\omega\left(4n(n-1)H_{n-2}(s) - 4nsH_{n-1}(s) + (s^2-1)H_n(s)\right)e(s) \\ &= \alpha\omega\left(4n(n-1)H_{n-2}(s) - 2n\left(H_n(s) + 2(n-1)H_{n-2}(s)\right) + \left(s^2-1\right)H_n(s)\right)e(s) \\ &= \alpha\omega\left(s^2 - 1 - 2n\right)H_n(s)e(s)\end{aligned} \tag{106}$$

We have in the latter step used equation 3 to find H_{n-1}.
We reuse the notation and differentiation from equation 106 and find the first derivatives to be

$$\begin{aligned}\sqrt{\alpha\omega}\frac{\partial}{\partial s}\left(H_n(s)e(s)\right) &= \sqrt{\alpha\omega}\left(\frac{\partial H_n}{\partial s} - sH_n\right)e(s) \\ &= \sqrt{\alpha\omega}\left(2nH_{n-1} - sH_n\right)e(s) \\ &= \sqrt{\alpha\omega}\left(2n\frac{H_{n-1}}{H_n} - s\right)H_n(s)e(s)\end{aligned} \tag{107}$$

The ratios for the one-body part are thus

$$\begin{aligned}\frac{\nabla\det(\Phi)}{\det(\Phi)} &= \sum_{k,j=1}^{N} \nabla_k \phi_j\left(\vec{r}_k, \alpha\right)\phi_{jk}^{-1}\left(\vec{r}, \alpha\right) \\ &= \sum_{k,j=1}^{N}\left(2\sqrt{\alpha\omega}\left(n_{x_j}\frac{H_{n_{x_j}-1}\left(\sqrt{\alpha\omega}x_k\right)}{H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_k\right)}\right) - \alpha\omega x_k, 2\sqrt{\alpha\omega}\left(n_{y_j}\frac{H_{n_{y_j}-1}\left(\sqrt{\alpha\omega}y_k\right)}{H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_k\right)}\right) - \alpha\omega y_k\right)\Phi_{kj}\Phi_{jk}^{-1}\end{aligned} \tag{108}$$

and the Laplacian

$$\begin{aligned}\frac{\nabla^2\det(\Phi)}{\det(\Phi)} &= \sum_{k,j=1}^{N} \nabla_k^2 \phi_j\left(\vec{r}_k, \alpha\right)\phi_{jk}^{-1}\left(\vec{r}, \alpha\right) \\ &= \alpha\omega\sum_{k,j=1}^{N}\left(\alpha^2\omega^2 r_k^2 - 2\left(n_{x_j} + n_{y_j} + 1\right)\right)\Phi_{kj}\Phi_{jk}^{-1}\end{aligned} \tag{109}$$

For the Jastrow-factor we need the derivatives to the function in the exponent. Label this f_{ij} and find

$$\begin{aligned}\frac{\partial f_{ij}}{\partial r_{ij}} &= \frac{\partial}{\partial r_{ij}}\left(\frac{a}{\beta + \frac{1}{r_{ij}}}\right) \\ &= \frac{a}{\left(1 + \beta r_{ij}\right)^2}\end{aligned} \tag{110}$$

and

$$\frac{\partial^2 f_{ij}}{\partial {r_{ij}}^2} = -\frac{2a\beta}{\left(1+\beta r_{ij}\right)^3} \tag{111}$$

Giving the first derivative and the Laplacian of the Jastrow-factor(with equation 71)

$$\begin{aligned}\frac{\nabla g(\vec{r},\beta)}{g(\vec{r},\beta)} &= \sum_{i=1}^{k-1} \frac{a\left(\vec{r}_i - \vec{r}_k\right)}{r_{ik}\left(1+\beta r_{ik}\right)^2} - \sum_{i=k+1}^{N} \frac{a\left(\vec{r}_k - \vec{r}_i\right)}{r_{ki}\left(1+\beta r_{ki}\right)^2} \\ &= \sum_{i\neq k} \frac{a\left(\vec{r}_k - \vec{r}_i\right)}{r_{ki}\left(1+\beta r_{ki}\right)^2}\end{aligned} \tag{112}$$

and the Laplacian is (with equation 72)

$$\frac{\nabla^2 g(\vec{r},\beta)}{g(\vec{r},\beta)} = \sum_{i,j\neq k} \frac{\vec{r}_{ki}\cdot\vec{r}_{kj}}{r_{ki}r_{kj}} \frac{a_{ki}a_{kj}}{\left(1+\beta r_{ki}\right)^2\left(1+\beta r_{kj}\right)^2} + \sum_{j\neq k} \frac{a_{kj}}{r_{kj}\left(1+\beta r_{kj}\right)^2}\left(\frac{1}{r_{kj}} - \frac{2\beta}{1+\beta r_{kj}}\right) \tag{113}$$

and the local energy is thus

$$\begin{aligned}E_L &= \frac{1}{2}\sum_{k=1}^{N}\left(\omega^2 r_k^2 - \frac{\nabla_k^2\psi_T}{\psi_T}\right) + \sum_{i<j}\frac{1}{r_{ij}} \\ &= \frac{1}{2}\sum_{k=1}^{N}\left(\omega^2 r_k^2 - \frac{\nabla_k^2 \det(\Phi(\vec{r},\alpha))}{\det(\Phi(\vec{r},\alpha))} - \frac{\nabla_k^2 g(\vec{r},\beta)}{g(\vec{r},\beta)} - 2\frac{\nabla_k \det(\Phi(\vec{r},\alpha))}{\det(\Phi(\vec{r},\alpha))}\cdot\frac{\nabla_k g(\vec{r},\beta)}{g(\vec{r},\beta)}\right) + \sum_{i<j}\frac{1}{r_{ij}}\end{aligned} \tag{114}$$

VII.B ANALYTIC EXPRESSION FOR DERIVATIVES OF VARIATIONAL PARAMETERS

The first derivatives of the wave function with respect to the variational parameters is needed in order to minimize with gradient descent method as described in section II.D. We solve the derivatives generally for a variational parameters c_n. The first derivative is thus

$$\begin{aligned}\frac{\partial\langle E_L\rangle}{\partial c_n} &= \frac{\partial}{\partial c_n}\left(\int \frac{\psi_T^2 E_L}{\int\psi_T^2 \mathrm{d}\tau}\right) \\ &= \int\left(\frac{\int\psi_T^2\mathrm{d}\tau\left(2\psi_T E_L\frac{\partial\psi_T}{\partial c_n} + \psi_T^2\frac{\partial E_L}{\partial c_n}\right) - 2\psi_T^2 E_L\int\psi_T\frac{\partial\psi_T}{\partial c_n}\mathrm{d}\tau}{\left(\int\psi_T^2\mathrm{d}\tau\right)^2}\right)\mathrm{d}\tau \\ &= 2\left\langle\frac{E_L}{\psi_T}\frac{\partial\psi_T}{\partial c_n}\right\rangle - 2\langle E_L\rangle\left\langle\frac{1}{\psi_T}\frac{\partial\psi_T}{\partial c_n}\right\rangle\end{aligned} \tag{115}$$

In the last step the hermiticity of the Hamiltonian was used. We have also used the fact that the trial wave function ψ_T is a real function.

For the derivative of the wavefunction, we find the elements individually by using Jacobi's formula as described in section II.G. We see that we need to first find the derivative to the individual elements in Φ. These are found by using the product rule, but we also see that we need the derivative to the individual Hermite polynomials. These are simply (with the chain rule)

$$\begin{aligned}\frac{\partial}{\partial x_i}H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right) &= \frac{x_i}{2}\sqrt{\frac{\omega}{\alpha}}\frac{\partial H_{n_{x_j}}}{\partial x_i} \\ &= n_{x_j}x_i\sqrt{\frac{\omega}{\alpha}}H_{n_{x_j}-1}\left(\sqrt{\alpha\omega}x_i\right) \\ &= \frac{n_{x_j}}{2\alpha}\left(1 + x_i\sqrt{\frac{\omega}{\alpha}}\left(n_{x_j}-1\right)\frac{H_{n_{x_j}-2}\left(\sqrt{\alpha\omega}x_i\right)}{H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right)}\right)H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right)\end{aligned} \tag{116}$$

The same differentiation is valid for $H_{n_{y_j}}$ as well. In the latter step we used equation 3. The first derivative of Φ_{ij} with respect to α is thus

$$\begin{aligned}\frac{\partial\Phi_{ij}}{\partial\alpha} &= \frac{\partial}{\partial\alpha}\left(H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right)H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_i\right)\exp\left(-\frac{\alpha\omega}{2}r_i^2\right)\right) \\ &= \left(H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_i\right)\frac{\partial}{\partial\alpha}H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right) + H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right)\frac{\partial}{\partial\alpha}H_{n_{y_j}}\left(\sqrt{\alpha\omega}y_i\right) - \frac{\omega r_i^2}{2}\right)\exp\left(-\frac{\alpha\omega}{2}r_i^2\right) \\ &= \frac{1}{2}\left(\Theta_{ij}(\alpha,x) + \Theta_{ij}(\alpha,y) - \omega r_i^2\right)\Phi_{ij}\end{aligned} \tag{117}$$

with

$$\Theta_{ij}(\alpha,x)\equiv\frac{n_{x_j}}{\alpha}\left(1+x_i\sqrt{\frac{\omega}{\alpha}}\left(n_{x_j}-1\right)\frac{H_{n_{x_j}-2}\left(\sqrt{\alpha\omega}x_i\right)}{H_{n_{x_j}}\left(\sqrt{\alpha\omega}x_i\right)}\right) \tag{118}$$

Using Jacobi's formula the first derivative with respect to α of ψ_T is

$$\begin{aligned}\frac{\partial\psi_T}{\partial\alpha}&=g\left(\vec{r},\beta\right)\frac{\partial}{\partial\alpha}\left(\det(\Phi)\right)\\&=g\left(\vec{r},\beta\right)\mathrm{Tr}\left(\mathrm{adj}\left(\Phi\right)\frac{\partial\Phi}{\partial\alpha}\right)\\&=g\left(\vec{r},\beta\right)\det(\Phi)\sum_{i,j=1}^{N}\Phi_{ij}^{-1}\frac{\partial\Phi_{ji}}{\partial\alpha}\\&=\frac{\psi_T}{2}\sum_{i,j=1}^{N}\Phi_{ij}^{-1}\Phi_{ji}\left(\left(\Theta_{ji}(\alpha,x)+\Theta_{ji}(\alpha,y)\right)-\omega r_j^2\right)\end{aligned} \tag{119}$$

where we have used equations 28 and 118.
The derivative with respect to β follows a similar approach as in section VII.A.2 giving

$$\begin{aligned}\frac{\partial\psi_T}{\partial\beta}&=\det(\Phi\left(\vec{r},\alpha\right))\frac{\partial}{\partial\beta}\left(\prod_{i<j}\exp\left(\frac{a}{\beta+\frac{1}{r_{ij}}}\right)\right)\\&=\det(\Phi\left(\vec{r},\alpha\right))g\left(\vec{r},\beta\right)\frac{\partial}{\partial\beta}\left(\sum_{i<j}\frac{a}{\beta+\frac{1}{r_{ij}}}\right)\\&=-\psi_T\sum_{i\neq j}\frac{a}{\left(\beta+\frac{1}{r_{ij}}\right)^2}\end{aligned} \tag{120}$$

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