# Project 1, Fys 4411

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## Contents



## Abstract

blablabla

# 1 Quantum dots

Our system of choice

# 2 The Monte Carlo method

## 2.1 Introduction

Monte Carlo (MC) methods includes a wide range of computational methods for solving integrals. The main idea is to sample the integrand $f(\mathbf{r})$ in random points $\{\mathbf{r}_i\}$, and finding an approximate solution to the integral by doing statistical analysis on the sampling data. The statistical error will give us an immediate idea of the precision of the result.

In general, any integral can be written on the form

$$\int_{\mathcal{D}} f(\mathbf{r})d\mathbf{r} = \int_{\mathcal{D}} P(\mathbf{r})g(\mathbf{r})d\mathbf{r}, \tag{1}$$

where $P(\mathbf{r})$ is a probability distribution. The integral can now be approximated by the sum

$$\int_{\mathcal{D}} f(\mathbf{r})d\mathbf{r} \approx \frac{1}{N}\sum_{i=1}^{N} g(\mathbf{r}_i), \tag{2}$$

where $\{\mathbf{r}_i\}$ is a set of random numbers drawn from the statistical distribution $P(\mathbf{r})$.

The simplest example, possible whenever the region of the of the integral is finite, is when $P$ is a uniform distribution bounded by the integration limits. Then $P(\mathbf{r})$ is a constant and $g(\mathbf{r}) = f(\mathbf{r})$. However, for many integrals this method will converge slowly and will require a very large number of samples to give accurate results. By choosing a

smart $P(\mathbf{r})$ that is large in the regions of interest, more samples will be drawn from the important regions, often leading to a more rapid convergence.

## 2.2 Markov Chain Monte Carlo

Markov Chain Monte Carlo (MCMC) provides us with a method for drawing the correct samples from $P$. Instead of drawing uncorrelated random samples we use a markow chain to generate a sequence $\{\mathbf{r}_n\}$ of vectors. A Markov chain is characterized by a transition kernel $q(\mathbf{x}|\mathbf{y})$ which is a probability density distribution of the variable $\mathbf{y}$, and which tells us the probability of a transition from $\mathbf{x}$ to $\mathbf{y}$. For each $\mathbf{r}_n$, we draw a new $\mathbf{r}_{n+1}$ from the distribution $q(\mathbf{r}_n, \mathbf{y})$. The distribution of the vectors in the set $\{\mathbf{r}_n\}$ will converge towards the distribution $P$ if the following conditions are fulfilled (reference):

- $P$ is an invariant of the kernel $q(\mathbf{x}|\mathbf{y})$ in the sense that

$$\int_{\mathcal{D}} d\mathbf{r}_A \, P(\mathbf{r}_A) q(\mathbf{r}_A|\mathbf{r}_B) = P(\mathbf{r}_B), \qquad (3)$$

- The chain is ergodetic, which means that any point $\mathbf{r}_n$ is accessible in a finite number transitions from any starting point $\mathbf{r}_0$.

It is costumary to make the analogy to a set of $\lambda$ biased random walkers, where the density of walkers $P_w$ is (close to) stationary and proportional to $P$. This analogy is reasonable as long as the sequence $\{\mathbf{r}_n\}$ can be split into $\lambda$ subsequences $\{\mathbf{r}_n^\lambda\}$ which are (practically speaking) uncorrelated. Then one can equally well interpret the samples as $N$ samples from one markov chain, as $N/\lambda$ samples from $\lambda$ markov chains.

For $P_w$ to be stationary (), the population of walkers in any point $\mathbf{r}_A$ must be () constant,

$$\sum_n P_w(\mathbf{r}_A) q(\mathbf{r}_A|\mathbf{r}_n) \approx \sum_n P_w(\mathbf{r}_n) q(\mathbf{r}_n|\mathbf{r}_A) \qquad (4)$$

This equation resembles(") (3) since both equations states that the density is stationary. The condition of detailed balance

$$P_w(\mathbf{r}_A) q(\mathbf{r}_A|\mathbf{r}_B) = P_w(\mathbf{r}_B) q(\mathbf{r}_B|\mathbf{r}_A). \qquad (5)$$

assures that (4) is fulfilled. As long as the markow chain is ergodetic the walkers will have access to all regions of the integration domain.

## 2.3 Metropolis-Hasting algorithm

We will now outline a general algorithm for the movement of the random walkers that fulfills (5). We introduce new scalar field to our equation $\gamma(\mathbf{r}_A, \mathbf{r}_B)$, which is a measure of the probability of accepting a move from $\mathbf{r}_A$ to $\mathbf{r}_B$. We split our transition kernel in two parts

$$q(\mathbf{r}_A|\mathbf{r}_b) \rightarrow \gamma(\mathbf{r}_A|\mathbf{r}_b) g(\mathbf{r}_A|\mathbf{r}_b). \qquad (6)$$

I will refer to $g(r_A|r_B)$ as the suggestion density, and $\gamma(\mathbf{r}_A|\gamma\mathbf{r}_B)$ as the acceptance probability. We set

$$\begin{aligned} &\gamma(\mathbf{r}_B|\mathbf{r}_A) = 1 \text{ when} \\ &P_w(\mathbf{r}_A) g(\mathbf{r}_A|\mathbf{r}_B) > P_w(\mathbf{r}_B) g(\mathbf{r}_B|\mathbf{r}_A). \end{aligned} \qquad (7)$$

Then, by inserting this equations into (5), we get

$$\gamma(\mathbf{r}_A|\mathbf{r}_B) = min\left(\frac{P_w(\mathbf{r}_B) g(\mathbf{r}_B|\mathbf{r}_A)}{P_w(\mathbf{r}_A) g(\mathbf{r}_A|\mathbf{r}_B)}, 1\right) \qquad (8)$$

By making this choice for $\gamma$, (5) will be fulfilled and the sequence $\{r_i\}$ will sample $P$. Note that only the relative ratio between the left and the right hand side of (eq) are of interest to us. Therefore, $P$ does not have to be normalized. These equations are implemented in the well known Metropolis-Hastings algorithm as follows:

**loop**
  $\mathbf{r}_B \leftarrow$ random from distribution $g(\mathbf{r}_T|\mathbf{r}_B)$.
  $\mathcal{X} \leftarrow$ random uniform. ($\mathcal{X} \in (0, 1)$)
  Calculate $\gamma(\mathbf{r}_n|\mathbf{r}_T)$).
  **if** $\mathcal{X} \leq \gamma$ **then**
    $\mathbf{r}_{n+1} \leftarrow \mathbf{r}_T$
  **else**
    $\mathbf{r}_{n+1} \leftarrow \mathbf{r}_n$
  **end if**
  $n \leftarrow n + 1$
**end loop**

## 2.4 Choice of transition kernel

One possibility us to use a suggestion density $g(\mathbf{r}_n|\mathbf{r}_{n+1})$ that is symmetric around $\mathbf{r}_n$ along all axis. This method is referred to as brute force sampling. In this case $\gamma(\mathbf{r}_{n+1}|\mathbf{r}_n)$ can be expressed as

$$\gamma(\mathbf{r}_{n+1}|\vec{r}_n) = min\left(\frac{P_w(\mathbf{r}_{n+1})}{P_w(\mathbf{r}_n)}, 1\right) \qquad (9)$$

A common choice is to set

$$g(\mathbf{r}_n|\mathbf{r}_{n+1}) = l\left(\mathcal{U}(\mathbf{r}_{n+1}-\mathbf{r}_n) - \frac{1}{2}\right) \tag{10}$$

where $l$ is a constant which we will refer to as the step length, and $\mathcal{U}(\mathbf{r})$ is the uniform distribution

$$\mathcal{U}(\mathbf{r}) = \begin{cases} 1, \text{ if all } \mathbf{r}\cdot\mathbf{e}_i \in [0,1] \\ 0, \text{ otherwise} \end{cases}. \tag{11}$$

Here $\mathbf{e}_i$ is the unit vectors of $\mathcal{D}$. The step length $l$ will alter the number of accepted steps during a simulation, and will have an effect on the rate of convergence.

An other class of transition kernels makes use of our knowledge of the mathematical form of $P$ by using a suggestion density that is dependent on it. By solving the Fokker-Planck equation for the stationary distribution $P$ one can construct a transition kernel that in principle will sample $P$ perfectly without the Metropolis-Hastings accept/reject procedure [5, 8]. However, it is necessary to discretize the dynamical equations in time $t \to t_n = \Delta t n$, and an time step error arises leading to an imperfect sampling of $P$. The Metropolis-Hastings algorithm corrects this error by restoring detailed balance.

The suggestion density becomes [5]

$$g(\mathbf{r}_{n+1}|\mathbf{r}_n) = K\exp(-D\Delta t\frac{\nabla P(\mathbf{r}_n)}{P(\mathbf{r}_n)} + \mathbf{r}_{n+1} - \mathbf{r}_n)^2, \tag{12}$$

where $D$ is the diffusion constant originating from the Fokker-Planck equation and $K$ is a normalization constant. Samples from this density are generated using the Langevin equation on the form (ref HAMMOND) (exact ? or is this where the dt dependent error enters)

$$\mathbf{r}_{n+1} = \mathbf{r}_n + D\Delta t\frac{\nabla P(\mathbf{r}_n)}{P(\mathbf{r}_n)} + \sqrt{\Delta t}\mathcal{N}(\mathbf{r}_{n+1}-\mathbf{r}_n), \tag{13}$$

where $\mathcal{N}$ is a normal distribution with the variance $2D$. From this equation it is evident that a small $\Delta t$ will lead to a small average step length $|\mathbf{r}_{n+1}-\mathbf{r}_n|$. This might slow down the convergence of the system even though the acceptance rate will increase. In practice one has to experiment to find the optimal values for $\Delta t$ that gives a ((small time step error)) and a rapid convergence.

# 3 Statistical analysis of the data

The statistical error is defined as the standard deviation of a sample mean, and can be estimated using the formula [4]

$$err \approx \sqrt{\frac{1}{N}Var(\mathcal{M})}, \tag{14}$$

where $\mathcal{M}$ is a set of $N$ uncorrelated sample means.

The samples obtained in the MCMC simulations is heavily correlated, mainly because of the high correlation between succeeding configurations $\mathbf{R}$. We get an estimate of $err$ by dividing our data into $N_\tau = N/\tau$ bins of $\tau$ samples, and calculating the standard deviation of the $N_\tau$ mean values.

$$err(\tau) \approx \sqrt{\frac{\tau}{N_\tau}Var(\mathcal{M}_\tau)} = \sqrt{\frac{\tau}{N_\tau}\langle\mathcal{M}_\tau^2\rangle - \langle\mathcal{M}_\tau\rangle^2}. \tag{15}$$

This is a good estimate if 1) $\tau$ is large enough so that the means $\mathcal{M}_\tau$ are practically uncorrelated and 2) $N_\tau$ is large enough to give us a good statistical value. Starting with a small $\tau$, $err(\tau)$ will converge towards the correct statistical error as $\tau$ increases. This method is referred to as blocking analysis. Fig. (**??**) shows a plot of $err(\tau)$ for a simulation of a 6 particle quantum dot with an error close to $\pm 10^{-5}$ Hartrees. The time between two practically uncorrelated samples, when the curve $err(\tau)$ flattens, will be referred to as the correlation length.

# 4 Quantum monte Carlo

## 4.1 Introduction

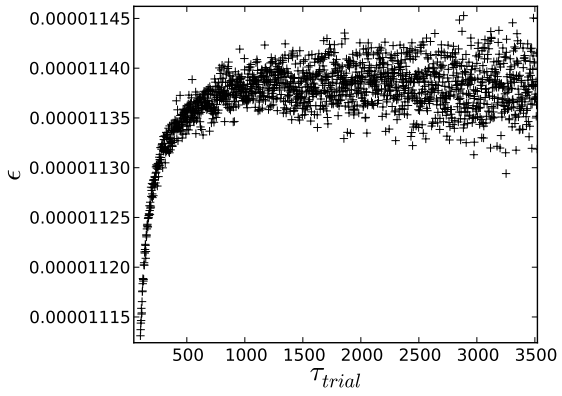
The expectation values of an observable $\hat{O}$ can be expressed on the general form

$$\langle O\rangle = \int d\mathbf{r}\Psi(\mathbf{r})\hat{O}\Psi(\mathbf{r})^*, \tag{16}$$

where $\Psi(\mathbf{r})$ is a solution to the schrödinger equation. The integral can also be written

$$\langle O\rangle = \int |\Psi(\mathbf{r})|^2\frac{\hat{O}\Psi(\mathbf{r})^\dagger}{\Psi(\mathbf{r})^\dagger}, \tag{17}$$

Figure 1: *Blocking results for a* 6 *particle quantum dot with* $\omega = 1$ *and* $\Delta t = 0.05$*. A total of* $10^8$ *samples has been used in the simulation. From the plot we can see that the statistical error is close to* $\pm 10^{-5}$ *Hartrees, and that the correlation length is of the order* $\mathcal{O}(10^3)$*.*




Since $|\Psi(\mathbf{r})|^2$ is a probability density distribution we see that

$$\langle O \rangle \approx \sum_{i=1}^{N} \frac{\hat{O}\Psi(\mathbf{r}_i)^\dagger}{\Psi(\mathbf{r}_i)^\dagger}, \tag{18}$$

where the set of numbers $\{\mathbf{r}_i\}$ are drawn from $|\Psi|^2$. This sum can be sampled using the Metropolis-Hastings algorithm with the acceptance probability

$$\gamma(r_i|r_i+1) = \frac{g(r_i|r_{i+1})\Psi(\mathbf{r}_i)|^2}{g(r_{i+1}|r_i)|\Psi(\mathbf{r}_{i+1})|^2}. \tag{19}$$

$g(r_i|r_{i+1})$ is the suggestion density as described earlier. Note that $\Psi$ does not need to be normalized in the above equations. This saves us a great deal of work since the normalization of most wave functions would have to be done numerically for every new trial function.

## 4.2 Transition kernels

Brute force sampling is implemented using the suggestion density eq. (10) and a acceptance probability

$$\gamma(\mathbf{R}_{n+1}|\mathbf{R}_n) = max\left(\frac{|\Psi(\mathbf{R}_{n+1})|^2}{|\Psi(\mathbf{R}_n)|^2}\,,\,1\right) \tag{20}$$

Importance sampling based on Langevin dynamics is implemented using the following equations. The gradient of $P \to |\Psi|^2$ is

$$\mathbf{F}_n = \frac{\nabla|\Psi(\mathbf{R}_n)|^2}{|\Psi(\mathbf{R}_n)|^2} = 2\frac{\nabla\Psi(\mathbf{R}_n)}{\Psi(\mathbf{R}_n)}, \tag{21}$$

and the diffusion constant $D$ can be shown to be $1/2$ in our dimensionless units(ref). Combining these two quantities with eq. (13) gives us an equation to sample the suggestion density eq. (12).

$$\mathbf{R}_{n+1} = \mathbf{R}_n + \Delta t\frac{\nabla\Psi(\mathbf{R}_n)}{\Psi(\mathbf{R}_n)} + \sqrt{\Delta t}\mathcal{N}(\mathbf{R}_{n+1} - \mathbf{R}_n). \tag{22}$$

The acceptance probability is found combining eq. (12) and eq. (8)

$$\gamma(\mathbf{R}_{n+1}|\mathbf{R}_n) = min\left(G(\mathbf{R}_{n+1},\mathbf{R}_n)\frac{|\Psi(\mathbf{R}_{n+1})|^2}{|\Psi(\mathbf{R}_n)|^2}\,,\,1\right) \tag{23}$$

where $G(\mathbf{R}_{n+1},\mathbf{R})$ is the greens function

$$G(\mathbf{R}_{n+1},\mathbf{R}_n) = e^{-\frac{1}{2}\left(\mathbf{F}_{n+1}+\mathbf{F}_n\right)} \times e^{\left(\frac{1}{4}\Delta t\left(\mathbf{F}_n-\mathbf{F}_{n+1}\right)+\mathbf{R}_n-\mathbf{R}_{n+1}\right)}. \tag{24}$$

## 4.3 Variational Monte Carlo

According to the ritz principle, the expectationvalue for the energy

$$\epsilon_0 \geq \langle\Psi_T|\hat{H}|\Psi_T\rangle\,\forall\,|\Psi_T\rangle \in \mathcal{H}. \tag{25}$$

This means that any expectation value $\langle\hat{H}\rangle$ sets an upper limit to the energy of the system. This principle allows us to perform a systematic search for the lowest $\langle\hat{H}\rangle$ using a set of trial wave functions $|\Psi_T(\alpha,\beta,\dots)\rangle$ where $\alpha,\beta,\dots$ are variational parameters.

The search in the parameter space $(\alpha,\beta,\dots)$ can be done by performing a number of MCMC calculations on a grid. More sophisticated methods are also in use, like the stochastic gradient approximation which will be described later in this text.

Since the variance $\langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2 = 0$ for the eigenfunctions of $\hat{H}$, the variance is a measure of how close $|\Psi_T,\alpha,\beta,\dots\rangle$ is to the 'true' ground state

wave function of the system. Even if the lowest energy obtained in our simulations will be closest to the ground state energy, the trial function with the lowest variance might be a better fit to the 'true' ground state wave function.

## 4.4 The trial wave functions

Our system is a closed shell model with the hamiltonian

$$\hat{H} = -\frac{\nabla^2}{2} + \omega|\mathbf{R}|^2 - \sum_{i<j}\frac{1}{r_{ij}}. \tag{26}$$

Here $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ is a vector containing the position of all electrons in the system. , and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between electron $i$ and electron $j$. The equations

$$\phi^{\alpha}_{n_x n_y}(\mathbf{r}_i) = H_{n_y}(\sqrt{\omega\alpha}y)H_{n_x}(\sqrt{\omega\alpha}x) \times \exp(-\frac{1}{2}\omega\alpha|\mathbf{r}_i|^2) \tag{27}$$

are the eigenstates for the hamiltonian eq. (26) when $\alpha = 1$. $H_n(x)$ is the Hermite polynomials and $\alpha$ is a variational parameter $\alpha \in [0, 1)$ which represents the "shielding" effect that occurs when more than one electron is present in the system. Since the electrons carry a negative charge, the efficient external potential seen by the individual particles will be lower than the actual external potential.

Our trial wave function can be written on the form

$$\Psi(\mathbf{R}) = \mathcal{D}^{\alpha}_{\downarrow}(\mathbf{R})\mathcal{D}^{\alpha}_{\uparrow}(\mathbf{R})\mathcal{J}^{\beta}(\mathbf{R}) \tag{28}$$

Here $\mathcal{D}_{\uparrow}(\mathbf{R})$is a slater determinant consisting of the one particle solutions eq. (27). Table 1 shows which orbitals that enters the slater determinant up to the 6'th full shell. The slater determinant automatically fulfills the Pauli principle stating that any wave function consisting of identical fermions must be antisymmetric w.r.t. the exchange of two particles. $\mathcal{D}^{\alpha}_{\downarrow}(\mathbf{R})$ is the corresponding determinant for the spin down states. Note that in the case of a spin dependent hamiltonian, $\mathcal{D}^{\alpha}_{\downarrow}\mathcal{D}^{\alpha}_{\uparrow}$ would have to be written as one single slater determinant to preserve the antisymmetry of the wavefunction. This is also the case for the open shell quantum dots since they can have a non zero net spin. $\mathcal{J}^{\beta}(\mathbf{R})$ is the Jastrow factor which removes the singularities

| Shell | Electrons | One particle orbitals |
|---|---|---|
| 1 | 2 | $\psi_{00}$ |
| 2 | 6 | $\psi_{10}$, $\psi_{01}$ |
| 3 | 12 | $\psi_{20}$, $\psi_{11}$, $\psi_{02}$ |
| 4 | 20 | $\psi_{30}$, $\psi_{21}$, $\psi_{12}$, $\psi_{03}$ |
| 5 | 30 | $\psi_{40}$, $\psi_{31}$, $\psi_{22}$, $\psi_{13}$, $\psi_{04}$ |
| 6 | 42 | $\psi_{50}$, $\psi_{41}$, $\psi_{32}$, $\psi_{23}$, $\psi_{14}$, $\psi_{05}$ |

Table 1: *This table shows the one particle orbitals that is part of the slater determinants. Only the first orbital state $\psi_{00}$ is needed to fill the first shell. This corresponds to a two electron quantum dot, one spin up and one spin down electron. The three first orbitals (six electrons) $\psi_{20}$, $\psi_{11}$, $\psi_{02}$ are needed to fill the second shell. Six orbitals (twelwe electrons) are needed to fill the third shell and so on.*

in $\hat{H}\Psi(\mathbf{R})$ at $\mathbf{r}_i = \mathbf{r}_j$ (ref). We use a Jastrow factor with one variational parameter $\beta$,

$$\mathcal{J}^{\beta}(\mathbf{R}) = \prod_{i<j}\mathcal{J}_{ij}$$
$$\mathcal{J}_{ij} = \exp\left(\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right) \tag{29}$$

$a_{ij} = 1$ if the spins of particle $i$ and $j$ are parallel and $a_{ij} = \frac{1}{3}$ if the spins are perpendicular. See ref. [5] for a detailed derivation of the Jastrow factor.

The wave functions $\psi^{\alpha}n_x, n_y(\mathbf{R})$ is $n+1$ times degenerated in the $n$'th energy level (starting at 0). In the $s$'th full shell we then have $2\sum_{a=1}^{s} a$ particles. The basis states used in the different energy levels are listed in table (1).

According to an article written by Tauts (ref tauts), the energy of the 2 particle $\omega = 1$ quantum dot should be exactly 3 Hartrees. The kinetic energy *** (e without the ) ($\hat{H} \rightarrow -\nabla^2/2$) of the slater matrices can be shown to be (ref,appendix): $2\omega$ Hartrees fo two particles, $10\omega$ Hartrees for 6 particles, $28\omega$ Hartrees for 12 particles and 60 Hartrees for 20 particles. (formula)?. We have used this values to validate the part of the code involving the slater matrices.

# 5 Minimization of the wave functions

The minimization was performed using the stocastic gradient approach (SGA) [2, 3, 7]. This is a stocastic procedure which minimizes the gradient of the energy using a large number of sampling points. The variational parameters are updated iteratively using the formula

$$(\alpha_{n+1}, \beta_{n+1}) = (\alpha_n, \beta_n) - \gamma_n (\partial_\alpha, \partial_\beta) \langle E_L \rangle \quad (30)$$

The variable steplength $\gamma_n$ is a system dependent parameter that must fulfill

$$\sum_{n=0}^{\infty} \gamma_n^2 < \sum_{n=0}^{\infty} \gamma_n = \infty,$$
$$\gamma_n > 0, \quad lim_{n\to\infty}\gamma_n \to 0. \quad (31)$$

The SGA is based on the Robbins-Monroe theorem which states that under certain mathematical conditions $\lim_{n\to\infty}(\alpha_n, \beta_n)$ (30) are guaranteed to converge towards the minima $(\alpha_{min}, \beta_{min})$. The mathematical conditions include (31) and some constraints on the objective function which is typically met by QMC wavefunctions. The basis for the theory is discussed in [7] with references to the original articles.

I have used a $\gamma_n$ on the form

$$\gamma_n = (k * n + l)^{-0.8}, \quad (32)$$

where $k$ and $l$ are parameters that is calculated as a function of the average values of $|\partial_\alpha \langle E_L \rangle|$ and $|\partial_\beta \langle E_L \rangle|$ during the first iterations. $l$ is initially chosen to be 0, and $k$ to be 1. There is one counter $n$ for each of the parameters $\alpha, \beta$ which is updated every time the gradient changes its sign. The reason for this is that it is assumed that whenever the gradient changes its sign, the system is close to it's minima[3].

The maximum step length is set to 0.1. This stabilizes the simulation during the initial phase when $\gamma_n$ is small and the step length might be large. After the thermalization phase $\gamma_n$ is chosen so that the average step length becomes much smaller than 0.1.

The approximate value of the gradient $(\partial_\alpha, \partial_\beta) \langle E_L \rangle$ is obtained during a short MC run where $m = \mathcal{O}(10)$ uncorrelated samples are collected. I have used $m$ different walkers that collect one sample each every iteration. I also tried to use one walker collecting $m$ samples every iteration, but the high correlation between the samples leads to bad results if the number of samples $m$ is much smaller than the correlation length ($\mathcal{O}(10^3)$). After my experience, using many uncorrelated walkers instead of one speeds up the convergence of the algorithm considerably.

See algorithm **??** for a detailed pseudo code.

The algorithm proved efficient when applied on the full shell quantum dots.The optimization of the two particle quantum dots is done in a few seconds, the six particle quantum dot in less than thirty seconds and the twelve particle QD in about four minutes. All with an statistical error close to $10^{-3}$.

Note that the optimization converges much faster than one can calculate the energy. For example, to optimize the two particle quantum dot with an error in the variational parameters $\sim 10^{-3}$, only a few hundred thousand samples is needed (see figure ?), with a minima that is accurate to $\mathcal{O}(10^{-5})$ Hartrees. To obtain the energy with an error $\sim 10^{-5}$ Hartrees about $10^8$ MC-samples are needed.

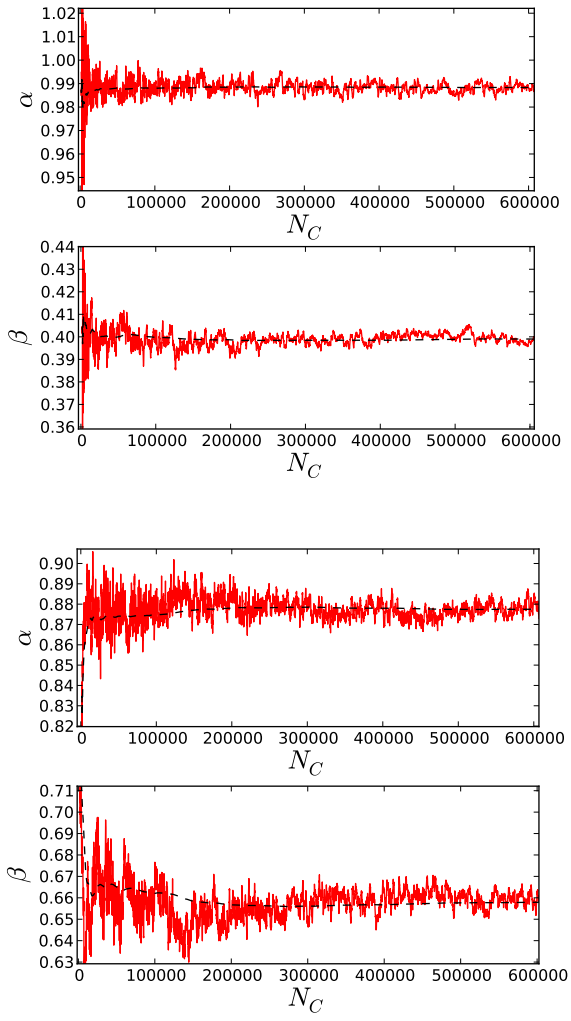
# 6 Implementation and optimization

The simulator can be efficiently optimized by implementing some mathematical shortcuts. The optimalizations can only be done if we only change the position of one electron at the time. The metropolis-hastings test is performed each cycle, while the energy and other observables are updated when we have cycled through all electrons. It would also be possible to evaluate the energy every time a electron has been moved, but this would not be favorable for a system with many electrons since the correlation between the samples would be very high, and the evaluation of the energy consumes too many flops.

## 6.1 Random number generators

I have used the random number generator `DRanNormalZig32` for generating normal distributed random numbers and `DRan_MWC8222` for generating uniformly distributes random numbers.

Figure 2: *Minimization of a* 6 *particle (top) and a* 12 *particle (bottom) quantum dot using an* $\omega = 1$ *and a* $\delta t = 0.05$. $N_C$ *is the total number of MC-samples. The red line shows the* $\alpha$ *and* $\beta$ *values at* $N_C$*, while the black line shows the accumulated mean. The means are quickly converging towards the optimal results (*$\beta = 0.399$, $\alpha = 0.988$*) (top) and (*$\beta = 0.877$, $\alpha = 0.657$*) (bottom), only using a total of total of* $6 \times 10^5$ *samples.*




The random number generators are programmed by Jurgen A. Doornik [1].

## 6.2 The update algorithm

## 6.3 Optimalization of $\mathcal{D}^\alpha(\mathbf{R})$

The inverse $D^{-1}$ of a matric $D$ can be written as the cofactor matrix $C/|D|$. $C$ has the elements $C_{ij} = |S_{ij}|$ where $S_{ij}$ is a sub matrix of $D$ with the $i$'th row and the $j$'th coloumn removed. The determinant $|D|$ can be expressed as

$$1 = \sum_j D_{ij} D^{-1}_{ji} = \sum_j D_{ij} \frac{C_{ji}}{|D|}$$
$$\Rightarrow \sum_j D_{ij} C_{ji} = |D| \tag{33}$$

From the definition of $C_{ij}$, we see that the $i$'th coloumn of $D^{-1} = C/|D|$ is unchanged if we change the $i$'th row of $D$. Therefore,

$$\text{if } D'_{ij} = D_{ij} \forall i \neq k$$
$$\sum_k D'_{kj} D'^{-1}_{jk} = \sum_k D'_{kj} D^{-1}_{jk} = \sum_k D'_{kj} \frac{C^{-1}_{jk}}{|D|}$$
$$\Rightarrow \sum_k D'_{kj} D'^{-1}_{jk} = \frac{|D'|}{|D|} \tag{34}$$

This operation scales much better than alternative ways of evaluation the determinant. For example ... The problem is that we need to obtain an expression for the inverse matrix $D^{-1}$. By using ... (ref) formula for updating the inverse matrix, we only need to evaluate the inverse matrix once. Updating the matrix scales as ...

Eq. (34) can be used to calculate the ratios

$$\frac{\mathcal{D}^\alpha(\mathbf{R}')}{D^\alpha(\mathbf{R})} = \sum_{ij} (\mathcal{D}_{ij}) \mathcal{D}^{-1}_{ji} \tag{35}$$
$$\frac{\nabla^2 \mathcal{D}^\alpha(\mathbf{R})}{D^\alpha(\mathbf{R})} = \sum_{ij} (\partial^2_{r_i} \mathcal{D}_{ij}) \mathcal{D}^{-1}_{ji} \tag{36}$$
$$\frac{\nabla_i \mathcal{D}^\alpha(\mathbf{R})}{D^\alpha(\mathbf{R})} = \sum_{j} (\partial_{r_i} \mathcal{D}_{ij}) \mathcal{D}^{-1}_{ji} \tag{37}$$

since all expressions can be written as a sum of slater determinants where only one row is changed. $\mathbf{R}'$ is equal to $\mathbf{R}$ except for the coordinates of one electron. The expressions for $\partial_{r_i} \mathcal{D}_{ij}$ and $\partial^2_{r_i} \mathcal{D}_{ij}$ is

calculated by evaluating the analytical expressions

$$\begin{aligned}\partial^2_{r_i}\mathcal{D}_{ij} &= \psi_{n_{xi},n_{yi}}((x_j,y_j),\alpha)\,\omega\alpha \\ &\left(\frac{\omega}{2}(x_j^2+y_j^2)-2\right. \\ &+4n_{xi}(n_{xi}-1)\frac{H_{n_{xi}-2}(\sqrt{\omega\alpha}x_j)}{H_{n_{xi}}(\sqrt{\omega\alpha}x_j)} \\ &+4n_{yi}(n_{yi}-1)\frac{H_{n_{yi}-2}(\sqrt{\omega\alpha}y_j)}{H_{n_{yi}}(\sqrt{\omega\alpha}y_j)} \\ &-4x\sqrt{\omega\alpha}\,n_{xi}\frac{H_{n_{xi}-1}(\sqrt{\omega\alpha}x_j)}{H_{n_{xi}}(\sqrt{\omega\alpha}x_j)} \\ &\left.-4y\sqrt{\omega\alpha}\,n_{yi}\frac{H_{n_{yi}-1}(\sqrt{\omega\alpha}y_j)}{H_{n_{yi}}(\sqrt{\omega\alpha}y_j)}\right) \qquad (38)\end{aligned}$$

$$\begin{aligned}\partial_{r_i}\mathcal{D}_{ij} &= \psi_{n_{xi},n_{yi}}((x_j,y_j),\alpha) \\ &\left(\mathbf{e}_x(2n_{xi}\sqrt{\omega\alpha}\frac{H_{n_{xi}-1}(\sqrt{\omega\alpha}x_j)}{H_{n_{xi}}(\sqrt{\omega\alpha}x_j)}-x\omega\alpha)\right. \\ &\left.\mathbf{e}_y(2n_{yi}\sqrt{\omega\alpha}\frac{H_{n_{yi}-1}(\sqrt{\omega\alpha}y_j)}{H_{n_{yi}}(\sqrt{\omega\alpha}y_j)}-y\omega\alpha)\right) \qquad (39)\end{aligned}$$

The expressions is derived using the same strategy as we have used when $(\partial_\alpha)\psi_i(\mathbf{r}_j)$ is derived in appendix A. The full derivation is found in [5]. When only one particle is updated, only one of the determinants $\mathcal{D}_\downarrow$, $\mathcal{D}_\uparrow$ needs to be evaluated since ... Analytical vs. numerical derivatives.

## 6.4 Optimalization of $\mathcal{J}^\beta(\mathbf{R})$ and $r_{ij}$

There are only $n(n-1)/2$ distinct values of $r_{ij}$. Therefore, all values can be stored in a lower tridiaginal matric with zeros on the diagonal.

$$P=\begin{pmatrix}0 & 0 & 0 & \dots\\ r_{21} & 0 & 0 & \\ r_{31} & r_{32} & 0 & \\ r_{41} & r_{42} & r_{43} & \\ \vdots & & & \end{pmatrix} \qquad (40)$$

If we move one electron, only $(n-1)$ elements has to be updated.

The electron-electron potential can be directly calculated by summing the $(n-1)$ inverse elements of $P$. The Jastrow ratio can be calculated

$$\frac{\mathcal{J}^\beta(\mathbf{R}')}{\mathcal{J}^\beta(\mathbf{R})}=\prod_{i=k \text{ or } j=k}\frac{\mathcal{J}^\beta_{ij}(\mathbf{R}')}{\mathcal{J}^\beta_{ij}(\mathbf{R})} \qquad (41)$$

when only the electron with coordinates $\mathbf{r}_k$ has been moved. This expression can be efficiently evaluated as the exponential of the sum of $2(n-1)$ elements

$$\begin{aligned}\frac{\mathcal{J}^\beta(\mathbf{R}')}{\mathcal{J}^\beta(\mathbf{R})} &= \exp\left(\sum_{i=k \text{ or } j=k} j(r_{ij})-j(r'_{ij})\right) \\ j(r_{ij}) &= \frac{a_{ij}r_{ij}}{1+\beta r_{ij}}. \qquad (42)\end{aligned}$$

The laplacian and the gradient .. can be evaluated ... the gradient: subltract $n-1$ old values, add $n-1$ new values.

## 6.5 Optimalization of $(\partial_\alpha,\partial_\beta)\langle E_L\rangle$

The gradient are calculated using an analytical expression for the energy. [6]

$$\begin{aligned}&(\partial_\alpha,\partial_\beta)\langle E_L\rangle = \\ &2\Big\langle\frac{(\partial_\alpha,\partial_\beta)\Psi}{\Psi}E_L\Big\rangle-2\Big\langle\frac{(\partial_\alpha,\partial_\beta)\Psi}{\Psi}\Big\rangle\langle E_L\rangle, \qquad (43)\end{aligned}$$

where

$$\begin{aligned}&\frac{(\partial_\alpha,\partial_\beta)\Psi(\mathbf{R},\alpha,\beta)}{\Psi(\mathbf{R},\alpha,\beta)} \\ &=\left(\frac{\partial_\alpha\mathcal{D}(\mathbf{R},\alpha)}{\mathcal{D}(\mathbf{R},\alpha)},\frac{\partial_\beta\mathcal{J}(\mathbf{R},\beta)}{\mathcal{J}(\mathbf{R},\beta)}\right) \qquad (44)\end{aligned}$$

From the definition of the Jastrow eq. (..) we can derive

$$\frac{\partial_\beta\mathcal{J}(\mathbf{R},\beta)}{\mathcal{J}(\mathbf{R},\beta)}=\sum_{k<l}-a\left(\frac{r_{kl}}{1+\beta r_{kl}}.\right)^2 \qquad (45)$$

The expression is calculated as a sum over the relevant distances $r_{kl}=|\mathbf{r}_k-\mathbf{t}_l|$ which is already stored in the matrix $P$ (40). The gradient of alpha is calculated using the expression:

$$\frac{\partial_\alpha\mathcal{D}(\mathbf{R},\alpha)}{\mathcal{D}(\mathbf{R},\alpha)}=\sum_i\sum_j(\partial_\alpha\psi_i(\mathbf{r}_j,\alpha))\mathcal{D}^{-1}_{ji} \qquad (46)$$

$$\begin{aligned}&\partial_\alpha\psi_i(\mathbf{r}_j,\alpha) = \\ &\psi_{n_{xi},n_{yi}}((x_j,y_j),\alpha)\left(n_{xi}\sqrt{\frac{\omega}{\alpha}}\frac{H_{n_{xi}-1}(\sqrt{\omega\alpha}x_j)}{H_{n_{xi}}(\sqrt{\omega\alpha}x_j)}\right. \\ &\left.+n_{yi}\sqrt{\frac{\omega}{\alpha}}\frac{H_{n_{yi}-1}(\sqrt{\omega\alpha}y_j)}{H_{n_{yi}}(\sqrt{\omega\alpha}y_j)}-\frac{\omega}{2}(x_j^2+y_j^2)\right) \qquad (47)\end{aligned}$$

Here $r_j \rightarrow (x_j, y_j)$ and $i \rightarrow n_{xi}, n_{yi}$. The values $\partial_\alpha \psi_i(\mathbf{r}_j, \alpha)$ are already stored in the matrix $\mathcal{D}$, and does not have to be calculated. All of the analytical expressions above is derivated in appendix A.

# 7 Results

## 7.1 Scaling and time consume

I have used the package `GNU gprof` to profile my program.

The time spent on running the code for $n_p = \{2, 6, 12, 20\}$ particles is listed in table 2. A curve fit to this data indicates that the algorithm scales as $\mathcal{O}(n_p^{2.5})$.

In table 2 I have also listed the percentage of the total floating point operation spent on the three most expensive functions. The evaluation of the first derivatives of the single particle orbitals soon becomes the most time consuming part of the code. This part of the code scales bad since the mathematical expressions for the orbitals eq. (27) gets more complex as the orbital energies increases. The problem is that half of these derivatives are calculated each time one particle is moved. It is possible to store the values, reducing the number of analytical expressions that has to be calculated $n/2$ times (?). This did not pay off when I tried to implement it since the number of variables that has to be stored is too high $(1/2(n_p)^2$(*dim?) for our system). The copying and accessing of the elements when accepting or rejecting a move is simply too expensive.

**** This shows us how important it is to use the analytical derivatives to optimize the code. I did a test run with a two particle quantum with a total of $10^8$ sampling cycles. The cpu time spent calculating the first and second derivatives of the orbitals increased from 2s to 47s when using numerical instead of analytical derivatives.

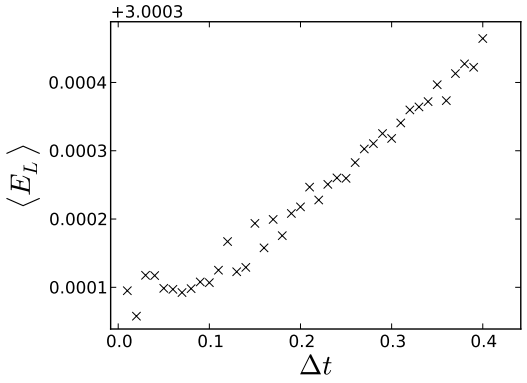
## 7.2 Systematic errors

Systematic time step error see HAMMOND (monte carlo methods in ab initio quantum chemistry)

## 7.3 Numerical results

The results are summarized in tables 3 and 4. I have used the values $\omega = 0.28, 0.5, 1.0$ and $\Delta t = 0.01, 0.25, 0.05$ to be able to compare my results with ref(...). I have also calculated the values using the same number of cycles. The results are well consistent with the results of (refLE),..

Figure 3: *Energy as a function of $\Delta t$ for a 2 particle quantum dot with $\alpha = 0.988, \beta = 0.399, \omega = 1$. All energies are calculated using $10^7$ samples. The energy are plotted for 40 values of $\Delta t$ between 0.01 and 0.4.*



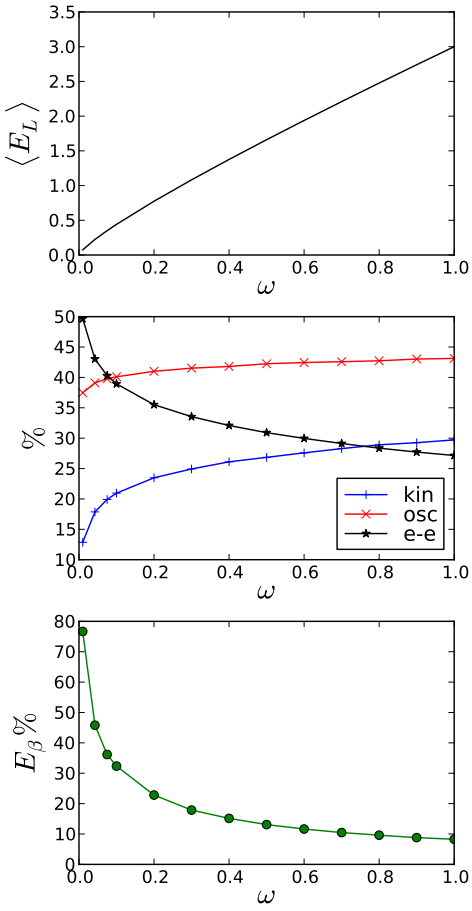

| $N_p$ | cpu time | d1 | jasgrad | slagrad |
|---|---|---|---|---|
| 2 | $1.1s$ | 4% | 10% | 6% |
| 6 | $8.5s$ | 10% | 16% | 14% |
| 12 | $37.8s$ | 20% | 14% | 13% |
| 20 | $135.3s$ | 37% | 11% | 16% |

Table 2: *Running time for $\omega = 1$ quantum dots with $N_p$ particles and the optimal values for the variational parameters. All runs done on one $2.4MHz$ processor with $10^6$ iterations. The percentage of time consume of the most expensive functions are listed in the table. (d1) :evaluation of the first derivatives of the orbitals, (jasgrad) :evaluation of the gradient of the Jastrow factor, (slagrad) :evaluation of the gradient of the Slater matrix (d1 not included).*

Speed tests.

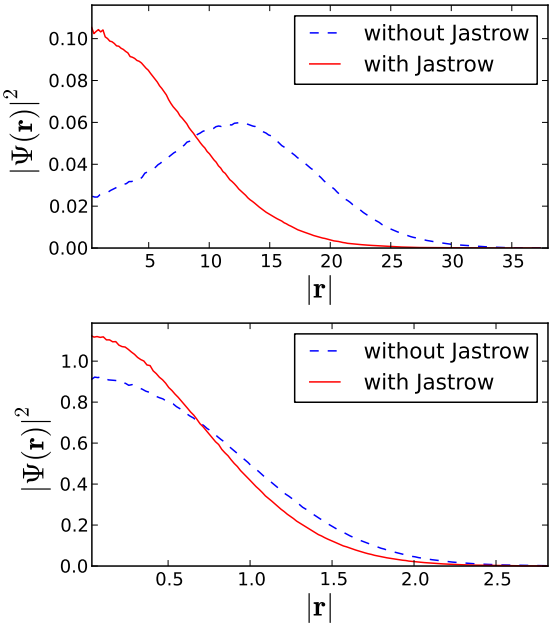
The timestep error: We have calculated all energy with three different values for $\Delta t$. The timestep error seems to be of the same order as the statistical error for our values of $\Delta t$. There is also a general trend in the variance and the statisti-

Figure 4: *Different quantities are plotted as a function of $\omega$ for a 2 particle quantum dot with the optimal variational parameters. All energies are calculated using $10^7$ samples and $\Delta t = 0.05$. Top plot: The total energy. Middle plot: Blue line ($-+$): kinetic energy, red line ($-\times$) oscillator potential energy, black line ($-*$) electron-electron potential energy. Percentage of total energy for each $\omega$ plotted. Bottom plot: The Jastrow energy as a percentage of the total energy. ((...) - $\langle E_L \rangle$ ) / $\langle E_L \rangle$.*




cal error as a function of $\Delta t$. The variance and the statistical error increases as $\Delta t$ gets smaller. The correlation length((plots?)) are generally increasing when $\Delta t$ gets smaller, probably explaining the increase in the variance and statistical error since the system will use a longer time to equilibriate after random fluctiations away from equilibrium (eg.

Figure 5: *The single particle densities for a two particle dot with $\omega = 1$ (top plot) and $\omega = 0.01$ (bottom plot). The single particle densities are calculated with and without the Jastrow function. These plots demonstrates that the correlation effects included in the Jastrow function are more important when $\omega$ gets small.*




if a sequence of mc-steps with a very low metropolis probability are accepted).

## 7.4 Verification of the results (literature,articles)

can see that the timestep error a

The SGA algorithm works well. First of all, it seems as the algorithm is working for different systems. Some parameter tuning seems inevitable for any new system. This can be solved by implementing some sort of line search along the gradient $\partial$.... One possibility is to implement a Newtonian approach to estimate the minima for each iteration. The hessian matrix can be evaluated analytically for each new configuration of the system [ref]. This approach has many advantages. In particular for

| $N_p$ | $\omega$ | $N_s$ | $\alpha_{min}$ | $\beta_{min}$ |
|---|---|---|---|---|
| 2 | 0.28 | $10^7$ | 0.971 | 0.252 |
| 2 | 0.5 | $10^7$ | 0.981 | 0.309 |
| 2 | 1 | $10^7$ | 0.988 | 0.399 |
| 6 | 0.28 | $10^7$ | 0.873 | 0.326 |
| 6 | 0.5 | $10^7$ | 0.900 | 0.413 |
| 6 | 1.0 | $10^7$ | 0.924 | 0.557 |
| 12 | 0.28 | $10^7$ | 0.809 | 0.378 |
| 12 | 0.5 | $10^7$ | 0.845 | 0.482 |
| 12 | 1.0 | $10^7$ | 0.877 | 0.658 |

Table 3: *Minimization results. $N_p$ is the number of particles and $N_s$ is the number of cycles used to obtain the energies and the gradient during the minimization. $\alpha_{min}$ and $\beta_{min}$ is the values of the variational parameters at the minima. We have used a $\Delta t = 0.05$ during the minimization.*

trial functions with asymmetrical minima, where the gradient is larger on one side of the minima then on the other. For an algorithm without an adaptive step size, the step length will have to be very small to give accurate results.

Two reasons: 1) mean value of variational parameters taken gives higher stability. The algorithm as it is implemented by (refs) Does not take the mean, but lets $\gamma$ increase faster to obtain a

# A Pseudocode: The SGA algorithm.

My implementation of the SGA. At $n = N_A/N_B$ start/stop collecting mean value of gradient. At $n = N_B$, $k, l$ is calculated. At $N_C$ the system should be thermalized and we start collecting data. $v_{min}$ is the lower limit of the variational parameters $\alpha, \beta$. $d_{max}$ is the upper limit for the length of a step in each variational parameter. $k, l$ are dependent on $D, E, F$. $E$ is the (negative) exponent limited by eq. (31). I have used $m = 30$, $N_A = 50$, $N_B = 120$, $N_C = 200$, $v_{min} = 0.01$, $d_{max} = 0.1$, $D = 300$, $E = 0.8$, $F = 20$ in all calculations.

**Initialize $m$ walkers**
$k_\alpha \leftarrow 0, l_\alpha \leftarrow 1$
$k_\beta \leftarrow 0, l_\beta \leftarrow 1$
**loop**

| $N_p$ | $\omega$ | $\Delta t$ | $N_s$ | $\langle E_L \rangle$ | $\sigma^2$ |
|---|---|---|---|---|---|
| 2 | 0.28 | 0.01 | $10^8$ | 1.02213(3) | 0.00076627 |
| 2 | 0.28 | 0.025 | $10^8$ | 1.02219(2) | 0.00075989 |
| 2 | 0.28 | 0.05 | $10^8$ | 1.02218(1) | 0.00076032 |
| 2 | 0.5 | 0.01 | $10^8$ | 1.66022(3) | 0.00116982 |
| 2 | 0.5 | 0.025 | $10^8$ | 1.66024(2) | 0.00116586 |
| 2 | 0.5 | 0.05 | $10^8$ | 1.66025(1) | 0.00116698 |
| 2 | 1.0 | 0.01 | $10^8$ | 3.00030(3) | 0.00183428 |
| 2 | 1.0 | 0.025 | $10^8$ | 3.00036(2) | 0.00182671 |
| 2 | 1.0 | 0.05 | $10^8$ | 3.00038(1) | 0.00182404 |
| 6 | 0.28 | 0.01 | $10^8$ | 7.6213(1) | 0.017831 |
| 6 | 0.28 | 0.025 | $10^8$ | 7.6214(1) | 0.017634 |
| 6 | 0.28 | 0.05 | $10^8$ | 7.6214(1) | 0.017383 |
| 6 | 0.5 | 0.01 | $10^8$ | 11.8100(2) | 0.043103 |
| 6 | 0.5 | 0.025 | $10^8$ | 11.8108(1) | 0.042331 |
| 6 | 0.5 | 0.05 | $10^8$ | 11.8101(1) | 0.041268 |
| 6 | 1.0 | 0.01 | $10^8$ | 20.1898(3) | 0.123116 |
| 6 | 1.0 | 0.025 | $10^8$ | 20.1904(2) | 0.119393.. |
| 6 | 1.0 | 0.05 | $10^8$ | 20.1905(1) | 0.115563 |
| 12 | 0.28 | 0.01 | $10^8$ | 25.6994(4) | 0.0621312 |
| 12 | 0.28 | 0.025 | $10^8$ | 25.6993(3) | 0.0611159 |
| 12 | 0.28 | 0.05 | $10^8$ | 25.6993(2) | 0.0599358 |
| 12 | 0.5 | 0.01 | $10^8$ | 39.2356(4) | 0.153526 |
| 12 | 0.5 | 0.025 | $10^8$ | 39.2345(3) | 0.149480 |
| 12 | 0.5 | 0.05 | $10^8$ | 39.2344(2) | 0.145622 |
| 12 | 1.0 | 0.01 | $10^8$ | 65.7908(5) | 0.441007 |
| 12 | 1.0 | 0.025 | $10^8$ | 65.7904(3) | 0.424902 |
| 12 | 1.0 | 0.05 | $10^8$ | 65.7903(2) | 0.409616 |

Table 4: *Monte carlo results using the variational parameters in table (3). Minimization results. $N_p$ is the number of particles and $N_s$ is the number of cycles used to obtain the energies and the gradient during the minimization. The thermalization is set to $5 \times 10^5$. The error is estimated using blocking analysis of the data.*

```
n = n + 1
for all walkers do
  propose new position for walker
  accept/reject move (metropolis test)
  sample (∂_α, ∂_β)E_L, E_L , (∂_α, ∂_β)E_L * E_L
end for
(∂_α, ∂_β)⟨E_L⟩ ← use eq. (43)
for ν = {α, β} do
  if n ∈ [N_A, N_B) then
    Δ_ν ← Δ_ν + |∂_ν⟨E_L⟩|
  end if
  if n = N_B then
    l_ν ← D^E(Δ_ν/(N_B − N_A))^{−E}
    k_ν ← l_ν/F
    n ← 0
  end if
  if |∂_ν⟨E_L⟩| > d_max then
    ν ← ν − d_max * ∂_ν⟨E_L⟩/|∂_ν⟨E_L⟩|
  else
    ν ← ν − ∂_ν⟨E_L⟩(k_ν * n + l_ν)^{−E}
  end if
  if ν < v_min then
    ν ← v_min
  end if
  if ∂_ν⟨E_L⟩ has changed its sign then
    n_ν ← n_ν + 1
  end if
end for
if n > N_C then
  accumulate mean values of α, β
end if
end loop
```

# B Derivation of the analytical expressions for $(\partial_\alpha, \partial_\beta)\langle \hat{H} \rangle$

The derivative of the jastrow factor can be written

$$\begin{aligned}\partial_\beta \mathcal{J}(\mathbf{R},\beta) &= \partial_\beta \prod_{i<j} \mathcal{J}_{ij}(\mathbf{R},\beta) \\ &= \sum_{k<l} \partial_\beta \mathcal{J}_{kl}(\mathbf{R},\beta) \prod_{i<j,(i,j)\neq(k,l)} \mathcal{J}_{ij}(\mathbf{R},\beta). \end{aligned} \quad (48)$$

We are interested in the ratio

$$\frac{\partial_\beta \mathcal{J}(\mathbf{R},\beta)}{\mathcal{J}(\mathbf{R},\beta)} = \frac{\partial_\beta \prod_{i<j} \mathcal{J}_{ij}(\mathbf{R},\beta)}{\prod_{i<j} \mathcal{J}_{ij}(\mathbf{R},\beta)} = \sum_{k<l} \frac{\partial_\beta \mathcal{J}_{kl}(\mathbf{R},\beta)}{\mathcal{J}_{kl}(\mathbf{R},\beta)}. \quad (49)$$

Evaluation of the terms $\delta_\beta \mathcal{J}_{kl}(\mathbf{R},\beta)$ is straight forvard, and the full expressions becomes

$$\frac{\partial_\beta \mathcal{J}(\mathbf{R},\beta)}{\mathcal{J}(\mathbf{R},\beta)} = \sum_{k<l} -a_{kl} \left( \frac{r_{kl}}{1+\beta r_{kl}} \right)^2. \quad (50)$$

The differention $\partial_\alpha \mathcal{D}(\mathbf{R},\alpha)$ can be written on the following form: (using partial derivation(???))

$$\begin{aligned}&\partial_\alpha \mathcal{D}(\mathbf{R},\alpha) \\ &= \begin{vmatrix} \partial_\alpha\psi_1(\mathbf{r}_1,\alpha) & \partial_\alpha\psi_1(\mathbf{r}_2,\alpha) & \partial_\alpha\psi_1(\mathbf{r}_3,\alpha) & \dots \\ \psi_2(\mathbf{r}_1,\alpha) & \psi_2(\mathbf{r}_2,\alpha) & \psi_2(\mathbf{r}_3,\alpha) & \\ \psi_3(\mathbf{r}_1,\alpha) & \psi_3(\mathbf{r}_2,\alpha) & \psi_3(\mathbf{r}_3,\alpha) & \\ \vdots & & & \end{vmatrix} \\ &+ \begin{vmatrix} \psi_1(\mathbf{r}_1,\alpha) & \psi_1(\mathbf{r}_2,\alpha) & \psi_1(\mathbf{r}_3,\alpha) & \dots \\ \partial_\alpha\psi_2(\mathbf{r}_1,\alpha) & \partial_\alpha\psi_2(\mathbf{r}_2,\alpha) & \partial_\alpha\psi_2(\mathbf{r}_3,\alpha) & \\ \psi_3(\mathbf{r}_1,\alpha) & \psi_3(\mathbf{r}_2,\alpha) & \psi_3(\mathbf{r}_3,\alpha) & \\ \vdots & & & \end{vmatrix} \\ &+ \dots \end{aligned} \quad (51)$$

$$= \mathcal{D}^{(1)}(\mathbf{r},\alpha) + \mathcal{D}^{(2)}(\mathbf{r},\alpha) + \dots \quad (52)$$

Since only one row in the determinant $\mathcal{D}^{(i)}(\mathbf{R},\alpha)$ is changed, following the same reasoning as in section ?.?, we can write

$$\frac{\mathcal{D}^{(i)}(\mathbf{R},\alpha)}{\mathcal{D}(\mathbf{R},\alpha)} = \sum_j (\partial_\alpha \psi_i(\mathbf{r}_j,\alpha)) \mathcal{D}^{-1}_{ji} \quad (53)$$

giving the expression

$$\frac{\partial_\alpha \mathcal{D}(\mathbf{R},\alpha)}{\mathcal{D}(\mathbf{R},\alpha)} = \sum_i \sum_j (\partial_\alpha \psi_i(\mathbf{r}_j,\alpha)) \mathcal{D}^{-1}_{ji}. \quad (54)$$

The terms $\partial_\alpha \psi_i(\mathbf{r}_j,\alpha)$ are derived below. We write $\psi_i(\mathbf{r}_j,\alpha) \rightarrow \psi_{n_{xi},n_{yi}}(\mathbf{r}_j,\alpha)$. where $n_{xi}$ and $n_{yi}$ is quantum numbers equal to or larger than zero.

$$\begin{aligned}&\psi_{n_{xi},n_{yi}}((x_i,y_i),\alpha) \\ &= H_{n_{xi}}(\sqrt{\omega\alpha}x_j) H_{n_{xi}}(\sqrt{\omega\alpha}x_j) \psi_{00}((x_i,y_i),\alpha) \end{aligned} \quad (55)$$

$H_n(x)$ is the hermite polynomials. Differentiation

gives

$$\partial_\alpha \psi_{n_{xi},n_{yi}}((x_i,y_i),\alpha) = \left(\partial_\alpha H_{n_{xi}}(\sqrt{\omega\alpha}x_j)\right)H_{n_{xi}}(\sqrt{\omega\alpha}x_j)\psi_{00}((x_i,y_i),\alpha) + H_{n_{xi}}(\sqrt{\omega\alpha}x_j)\left(\partial_\alpha H_{n_{xi}}(\sqrt{\omega\alpha}x_j)\right)\psi_{00}((x_i,y_i),\alpha) + H_{n_{xi}}(\sqrt{\omega\alpha}x_j)H_{n_{xi}}(\sqrt{\omega\alpha}x_j)\left(\partial_\alpha \psi_{00}((x_i,y_i),\alpha)\right) \tag{56}$$

We make use of the identity $\delta_x H_n(x) = 2nH_{n-1}(x)$,

$$\begin{aligned}\partial_\alpha H_n(\sqrt{\alpha\omega}x) &= \frac{\partial H_n(\sqrt{\alpha\omega}x)}{\partial(\sqrt{\alpha\omega}x)}\frac{\partial(\sqrt{\alpha\omega}x)}{\partial\alpha} \\ &= nx\sqrt{\frac{\omega}{\alpha}}H_{n-1}(\sqrt{\omega\alpha}x)\end{aligned} \tag{57}$$

Derivation of $\psi_{00}((x,y),\alpha)$ yields

$$\partial_\alpha \psi_{00}((x,y),\alpha) = -\frac{\omega}{2}(x^2+y^2)\psi_{00}((x,y),\alpha). \tag{58}$$

We combine eq. (56), eq. (57) and eq. (58)

$$\partial_\alpha \psi_i(\mathbf{r}_j,\alpha) = \psi_{n_{xi},n_{yi}}((x_j,y_j),\alpha)\left(x_j n_{xi}\sqrt{\frac{\omega}{\alpha}}\frac{H_{n_{xi}-1}(\sqrt{\omega\alpha}x_j)}{H_{n_{xi}}(\sqrt{\omega\alpha}x_j)} + y_j n_{yi}\sqrt{\frac{\omega}{\alpha}}\frac{H_{n_{yi}-1}(\sqrt{\omega\alpha}y_j)}{H_{n_{yi}}(\sqrt{\omega\alpha}y_j)} - \frac{\omega}{2}(x_j^2+y_j^2)\right) \tag{59}$$

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