FYS4411 - Project 1
Variational Monte Carlo

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Abstract

Abstract awesomeness

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2 Theoretical model

We investigate bosons in a potential trap. The Hamiltonian of such a system for N bosons is in general given by:

$$H = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{ext}(\boldsymbol{r}_i) \right) + \sum_{i<j}^{N} V_{int}(\boldsymbol{r}_i, \boldsymbol{r}_j) \tag{1}$$

Where V_{ext} is the external potential, i.e. the potential of the trap, whereas V_{int} is the interal potential, i.e. the potential between the bosons. We wish to approximate the ground state energy of our system described by the Hamiltonian given in equation 1.

2.1 The potentials employed

2.1.1 The external potential

We will focus on two different trap shapes: spherical and elliptical. The spherical trap can be described by a standard harmonic oscillator potential, which is given by:

$$V_{ext}(\boldsymbol{r}) = \frac{1}{2} m \omega_{ho}^2 r^2 \quad \text{(spherical trap)} \tag{2}$$

Where m is the mass of the bosons and ω_{ho} is a parameter characterizing the strength of the potential (the characteristic frequency of the trap). The elliptical trap, however, is given by:

$$V_{ext}(\boldsymbol{r}) = \frac{1}{2} m [\omega_{ho}^2 (x^2 + y^2) + \omega_z z^2] \quad \text{(elliptical trap)} \tag{3}$$

I.e. we allow the strength of the potential to vary in one direction, which we designate as the z-axis.

2.1.2 The internal potential

We will begin by investigating models where there is no repulsion between the bosons, however, we will later act a repulsive potential that prevents bosons from occupying the same point in space. With a as a typical diameter of our bosons (the hard-core diameter), we define our internal potential as:

$$V_{int}(|\boldsymbol{r}_i - \boldsymbol{r}_j|) = \begin{cases} \infty & |\boldsymbol{r}_i - \boldsymbol{r}_j| \leq a \\ 0 & |\boldsymbol{r}_i - \boldsymbol{r}_j| > a \end{cases} \tag{4}$$

This potential thus represents the impossibility of bosons to occupy the same point in space.

2.2 The variational method

2.2.1 The variational principle

To find the ground state energy, E_0 of bosons trapped in a potential, we employ the variational method. The variational principle states that:

$$E_0 \leq \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi | \Psi \rangle} \tag{5}$$

Where H is the Hamiltonian of our system and Ψ_T is any trial wavefunction. We therefore choose a functional form for Ψ_T, with a number of free parameters. By varying these parameteres, we can find an upper bound for the ground state energy. If our chosen functional form is reasonably close to the exact wavefunction, Ψ of the system, then our estimate for E_0 should be reasonably close to the actual ground state energy of our system.

2.2.2 Choosing a trial wavefunction

As noted above, we must choose our trial wavefunction to be reasonably close to the expected form of the actual position wavefunctions of our system. We note first that the external potential represents a harmonic oscillator. For the harmonic oscillator, it is well known from introductory quantum mechanics that the eigenfunctions are exponential functions for each particle seperately. Note that the elliptic oscillator has a preferred direction (the z-axis). We accomodate for this by introducing a parameter β, representing the asymmetry of the elliptical oscillator. We therefore choose our trial wavefunction for this part of the potential to be:

$$h(\boldsymbol{r}_1, ..., \boldsymbol{r}_N, \alpha, \beta) = \prod_{i=1}^{N} g(\alpha, \beta, \boldsymbol{r}_i) = \prod_{i=1}^{N} \exp\left[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right] = \exp\left[-\alpha \sum_{i=1}^{N} (x_i^2 + y_i^2 + \beta z_i^2)\right] \tag{6}$$

Where we now have two variational parameters, α and β. Here β tunes the strength of the potential as a whole, whereas β tunes the asymmetry of the spherical oscillator.

For the internal potential, we expect a function that attenuates our wavefunction down to zero if the distance between any pair of particles becomes less than a. We choose this function to be continuous, on physical grounds. A simple choice for such a function is:

$$f(a, |\boldsymbol{r}_i - \boldsymbol{r}_j|) = \begin{cases} 0 & |\boldsymbol{r}_i - \boldsymbol{r}_j| \leq a \\ 1 - \frac{a}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} & |\boldsymbol{r}_i - \boldsymbol{r}_j| > a \end{cases} \tag{7}$$

Putting this together, gives our trial wavefunction as:

$$\Psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N, \alpha, \beta) = \prod_i g(\alpha, \beta, \boldsymbol{r}_i) \prod_{i<j} f(a, |\boldsymbol{r}_i - \boldsymbol{r}_j|) \tag{8}$$

This is thus the wavefunction that we will be using in equation 5 to find our upper bound on the ground state energy.

2.3 Variational Monte Carlo

Note that equation 5 involves two integrals over $3N$ dimensions. This is usually not possible to evaluate analytically for large N, and traditional numerical methods such as gaussian quadrature are far too slow in high dimensions to be feasible. We therefore employ variational Monte Carlo methods to help in evaluting these integrals. To do this, we consider these integrals to represents stochastic quantities, and define the probability distribution as:

$$P(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N, \alpha, \beta) = \frac{|\Psi_T|^2}{\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 ... d\boldsymbol{r}_{\boldsymbol{n}} |\Psi_T|^2} \tag{9}$$

Now define a new quantity, the local energy, as:

$$E_L(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N, \alpha, \beta) = \frac{1}{\Psi_T} H \Psi_T \tag{10}$$

The expectation value of the Hamiltonian (i.e. the estimate of the energy) now turns into:

$$E[H(\alpha, \beta)] = \int P(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N, \alpha, \beta) E_L(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N, \alpha, \beta) d\boldsymbol{r}_1 d\boldsymbol{r}_2 ... d\boldsymbol{r}_N \approx \frac{1}{M} \sum_{i=1}^{M} E_{L,i} \tag{11}$$

Where now M is the number of Monte Carlo cycles, whereas $E_{L,i}$ is the local energy computed in the i-th Monte Carlo step. Note that the quality of this approximation is contingent upon our ability to sample our space. We employ two different algorithms for sampling our coordinate space.

2.3.1 The Metropolis algorithm

To move from one Monte Carlo step to the other, we will employ the Metropolis algorithm, as described in **REFERENCE**. The alogrithm works by sampling the probability distribution, but adding a bias to sample mostly in the regions where the probaility distribution actually is large, to avoid wasting CPU cycles. The algorithm works by proposing a step:

$$\boldsymbol{r}_{p,new} = \boldsymbol{r}_p + r \cdot \boldsymbol{dx} \tag{12}$$

Where r is a random number in $[0, 1]$ and $\boldsymbol{dx}$ is a chosen step vector. We then compute the ratio:

$$w = \frac{P(\boldsymbol{r}_1, ..., \boldsymbol{r}_{p,new}, ..., \boldsymbol{r}_n)}{P(\boldsymbol{r}_1, ..., \boldsymbol{r}_p, ..., \boldsymbol{r}_n)} = \frac{|\Psi_T(\boldsymbol{r}_1, ..., \boldsymbol{r}_{p,new}, ..., \boldsymbol{r}_n)|^2}{|\Psi_T(\boldsymbol{r}_1, ..., \boldsymbol{r}_p, ..., \boldsymbol{r}_n)|^2} \tag{13}$$

This ratio determines whether the new position has a higher or lower value of the PDF than the old position. We then accept the move if and only if $w \geq r$, where $r \in [0,1]$ is a uniformly distributed random variable. This ensures that some steps that decrease the value of the PDF are accepted (giving a spread of value), but that we mostly sample where the PDF is large (which avoids wasting CPU cycles).

2.3.2 The Metropolis-Hastings algorithm (importance sampling)

The simple Metropolis algorithm described above assigns no preferred direction $\boldsymbol{dx}$ for the proposed step. This can be improved by adding a force term, "pushing" the Monte Carlo loop towards the region where the PDF is large. This is described in further detail in **REFERENCE**, where it is shown that the expression fur such a quantum force is given, for particle k, by:

$$\boldsymbol{F}_k(\boldsymbol{r}_1, ..., \boldsymbol{r}_N) = 2\frac{1}{\Psi_T}\nabla_k \Psi_T \tag{14}$$

We compute explicitly the expression for $\boldsymbol{F}$, using the trial wavefunction in equation 8. This gives:

$$\boldsymbol{F} = \tag{15}$$

REMEMBER TO ADD THIS. A more detailed analysis (given in **REFERENCE**) shows that the correct way to incorporate such a term into the Metropolis algorithm is by adding a transition probability term given by the Green's functions:

$$G(\boldsymbol{r}_1, ..., \boldsymbol{r}_N, \boldsymbol{r'}_1, ..., \boldsymbol{r'}_N) = \frac{1}{(4\pi D\Delta t)^{3/2}} \sum_{i=1}^{N} \exp\left(- \frac{(\boldsymbol{r}_i - \boldsymbol{r'}_i - D\Delta t \boldsymbol{F}_i(\boldsymbol{r}_1, ..., \boldsymbol{r}_N))^2}{4D\Delta t} \right) \tag{16}$$

Where $\boldsymbol{r}_i$ are the coordinates prior to the move and $\boldsymbol{r'}_i$ are the coordinates after the move. The effect of this term is to modulate the acceptance probability, w. This term is now given by:

$$w(\boldsymbol{r}_1, ..., \boldsymbol{r}_N, \boldsymbol{r'}_1, ..., \boldsymbol{r'}_N) = \frac{G(\boldsymbol{r}_1, ..., \boldsymbol{r}_N, \boldsymbol{r'}_1, ..., \boldsymbol{r'}_N)|\Psi_T(\boldsymbol{r}_1, ..., \boldsymbol{r}_N)|^2}{G(\boldsymbol{r'}_N, ..., \boldsymbol{r}_1, ..., \boldsymbol{r}_N, \boldsymbol{r'}_1)|\Psi_T(\boldsymbol{r'}_1, ..., \boldsymbol{r'}_N)|^2} \tag{17}$$

Which leads to the modified Metropolis algorithm, the Metropolis-Hastings algorithm, where a move is accepted if and only if $w \geq r$ where $r \in [0,1]$ again is a uniformly distributed random variable. This method is computationally far more intensive, but leads to a larger number of accepted steps.

2.4 Gradient descent and conjugate gradient

3 Methods

3.1 Minimizing computation in the non-interacting case

For the non-interacting case ($a = 0$), certain shortcuts are possible, to save FLOPS.

3.1.1 Computing the numerical energy

From the Schrödinger equation:

$$\hat{H}\Psi_T = \left(-\frac{1}{2}\nabla^2 + V \right) \Psi_T = E\Psi_T \tag{18}$$

The kinetic energy is, numerically, given by (in dimensionless form):

$$T = -\frac{1}{2}\nabla^2 \Psi_T \tag{19}$$

This gives, for particle i and component j:

$$T_{ij} \approx \frac{\Psi_T(\boldsymbol{r_1}, ..., \boldsymbol{r_{i,j}} + h, ..., \boldsymbol{r_n}) - 2\Psi_T(\boldsymbol{r}) + \Psi_T(\boldsymbol{r_1}, ..., \boldsymbol{r_{i,j}} - h, ..., \boldsymbol{r_n})}{h^2} \tag{20}$$

Which gives, for the simplest trialfunction ($a = 0$):

$$T_{ij} = -\frac{1}{2}\Psi_T \left(\frac{\exp\big(-\alpha_j(x_j + h)^2\big)}{\exp\big(-\alpha_j x_j^2\big)} - 2 + \frac{\exp\big(-\alpha_j(x_j - h)^2\big)}{\exp\big(-\alpha_j x_j^2\big)} \right) \frac{1}{h^2} = -\frac{1}{2h^2}\Psi_T \left(\exp\big(-2\alpha_j x_j h - \alpha_j h^2\big) + \exp\big(2\alpha_j x_j h - \alpha_j h^2\big) \tag{21}$$

4 Results and discussion

5 Conclusion

5.1 Conclusion

5.2 Outlook

Appendices

A Finding the drift force

We wish to compute:

$$\vec{F} = 2\frac{1}{\psi_T}\nabla\psi_T \tag{22}$$

B Finding the analytic expression for the local energy

We wish to find:

$$E_L = \frac{1}{\Psi_T}\nabla^2\Psi_T \tag{23}$$

Where Ψ_T is given by:

$$\exp\left[-\alpha\sum_i^n \left(x_i^2 + y_i^2 + z_i^2\right)\right]\prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) \tag{24}$$

Look first at $a = 0$. In this case, this reduces to the harmonic oscillator potential. The local energy is then:

$$\exp\left[\alpha\sum_i^n \left(x_i^2 + y_i^2 + z_i^2\right)\right]\left(-\frac{\hbar^2}{2m_i}\nabla_i^2 + V\right)\exp\left[-\alpha\sum_i^n \left(x_i^2 + y_i^2 + z_i^2\right)\right] \tag{25}$$

In the simple harmonic oscillator case, this gives:

$$E_L(\mathbf{r}, \alpha) = -\frac{\hbar^2}{2m}\sum_{i=1}^n 2\alpha\left(2\alpha(x_i^2 + y_i^2 + z_i^2) - 3\right) + \frac{1}{2}m\omega_{ho}^2\sum_{i=1}^n (x_i^2 + y_i^2 + z_i^2) \tag{26}$$

FIX FOR ONE/N PARTICLES AND LOWER DIMENSION Similarly for the drift force:

$$F = \frac{2\nabla\Psi_T}{\Psi_T} \tag{27}$$

$$F = -2\alpha \sum_{i=1}^{n} (x_i + y_i + z_i) \tag{28}$$

Now for the ugly part:
For one particle, ∇_k:

$$\nabla_k \Psi_T = \nabla_k \left(\Psi_T(\mathbf{r}) = \nabla_k \prod_{i=1}^{n} \phi(\mathbf{r}_i) \exp\left(\sum_{i<j} u(r_{ij}) \right) \right) \tag{29}$$

Now apply the product rule. For the first term, all terms are unchanged except where $i = k$, giving the first term as:

$$\nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp\left(\sum_{i<j} u(r_{ij}) \right) \tag{30}$$

The second term is trickier. We can rewrite it as follows:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{i<j} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=1}^{n} \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] \tag{31}$$

This is calculated by using the chain-rule. To evaluate the innerfunction, we must look at $1 \leq j \leq k$, $j = k$ and $j \geq k$. Begining with $1 \leq j \leq k$, the first sum is from 1 up the kth particle, meaning all terms differentiated before k vanishes and we are left with $u(r_{ik})$, thus leaving with us with:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=1}^{k} \sum_{i=1}^{k-1} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{i=1}^{k-1} \nabla_k u(r_{ik}) \right] \tag{32}$$

For $j = k$, we see that the first sum goes from and end up at kth particle, meaning this sum vanishes, secondly, the second sum is evaluated at $1 \leq i \leq k-1$, leaving with constants up to $k-1$, thus this term becomes 0.

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=1}^{n} \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] = 0 \tag{33}$$

For $j > k$,the first sum goes from $k+1 \leq j \leq n$ and the second $1 \leq i \leq k$. The second sum vanishes, because all constants are differentiated away except the last term $i = k$. This leaves us with:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[\exp\left(\sum_{j=k+1}^{n} \sum_{i=1}^{k} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j=k+1}^{n} \nabla_k u(r_{kj}) \right] \tag{34}$$

We can now write the second term as 31):

$$\prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j=k+1}^{n} \nabla_k u(r_{kj}) + \left[\sum_{i=1}^{k-1} \nabla_k u(r_{ik}) \right] \right] \tag{35}$$

This can be rewritten to:

$$\prod_i \phi(\mathbf{r}_i) \exp\left\{ \left(\sum_{i<j} u(r_{ij}) \right) \right\} \left[\sum_{j \neq k} \nabla_k u(r_{kj}) \right] \tag{36}$$

FORKLAR denne delen litt. Thus the first derivative of the trial wavefunction can be written as:

$$\nabla_k \Psi_T = \nabla_k \phi(\mathbf{r}_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i)\right] \exp\left(\sum_{i<j} u(r_{ij})\right) + \prod_i \phi(\mathbf{r}_i) \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k u(r_{kj})\right] \tag{37}$$

Lastly we will calculate the second derivative of the trial function, where we use the product rule and the chain rule. We will then obtain the following:

$$\begin{aligned}\nabla_k^2 \Psi_T = &\underbrace{\nabla_k^2 \phi(\mathbf{r}_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i)\right] \exp\left(\sum_{i<j} u(r_{ij})\right)}_{\mathrm{I}} + \\ &\underbrace{2\left(\nabla_k \phi(\mathbf{r}_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i)\right] \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k u(r_{kj})\right]\right)}_{\mathrm{II}} + \\ &\underbrace{\prod_i \phi(\mathbf{r}_i) \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k u(r_{kj})\right]^2}_{\mathrm{III}} + \\ &\underbrace{\prod_i \phi(\mathbf{r}_i) \exp\left\{\left(\sum_{i<j} u(r_{ij})\right)\right\} \left[\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj})\right]}_{\mathrm{IV}}\end{aligned}$$

Where the derivatives of the different parts are obtained from previous. We will now divide the second derivative by the trial wavefunction, and obtain:

$$\frac{1}{\Psi_T}\nabla_k^2 \Psi_T = \underbrace{\frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_{\phi(\mathbf{r}_k)})}}_{\mathrm{I}} + \underbrace{2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{j\neq k} \nabla_k u(r_{kj})}_{\mathrm{II}} + \underbrace{\left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)^2}_{\mathrm{III}} + \underbrace{\left[\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj})\right]}_{\mathrm{IV}} \tag{38}$$

We will now carry out the differentiation in term (II), (III) and (IV). Begining with the (II), by using the chain rule we can rewrite (II) as:

$$2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{j\neq k} \frac{\partial u(r_{kj})}{\partial r_{kj}} \frac{\partial r_{kj}}{\partial \mathbf{r}_k} = 2\frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \left(\sum_{j\neq k} \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} u'(r_{kj})\right)$$

Where we have used $\nabla_k r_{kj} = (\mathbf{r}_k - \mathbf{r}_j)/r_{kj}$. Looking at (III), we can write out the square into two factors. The second paranthese the summation index is replaced by a dummy index i. Thus will look as:

$$\left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)^2 = \left(\sum_{j\neq k} \nabla_k u(r_{kj})\right) \left(\sum_{i\neq k} \nabla_k u(r_{ki})\right) \tag{39}$$

From (II) we found the derivative of this function. Thus this can be expressed as (combining also the double sum):

$$\left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)^2 = \sum_{i,j\neq k} \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right) \left(\frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}}\right) u'(r_{kj}) u'(r_{ki}) \tag{40}$$

The last part (IV), we must use the chain rule and product rule together. We will obtain the following term:

$$\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj}) = \sum_{j\neq k} \nabla_k \left(\left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right)^2 u''(r_{kj}) + u'(r_{kj}) \nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) \right) \tag{41}$$

Note that this is a unit vector squared:

$$\left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right)^2 = 1 \tag{42}$$

and the last part is found by using the qoutient rule. This is the divergence to the vectors, since we are evaluating for specific particle k, and gradient to scalar (we must look for all combination of k particle):

$$\nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) = \frac{r_{kj} \left(\nabla_k \cdot \mathbf{r}_k - \nabla_k \cdot \mathbf{r}_j \right) - (\mathbf{r}_k - \mathbf{r}_j) \nabla_k r_{kj}}{r_{kj}^2} \tag{43}$$

This simply becomes:

$$\nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) = \frac{3r_{kj}^2 - \mathbf{r}_k^2 + 2(\mathbf{r}_k \cdot \mathbf{r}_j) - \mathbf{r}_j^2}{r_{kj}^3} \tag{44}$$

Note that $r_{kj} - \mathbf{r}_k^2 + 2(\mathbf{r}_k \cdot \mathbf{r}_j) - \mathbf{r}_j^2 = 0$, this leaves us with:

$$\nabla_k \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) = \frac{2}{r_{kj}} \tag{45}$$

Thus expression (IV) can be expressed as:

$$\sum_{j\neq k} \nabla_k \nabla_k u(r_{kj}) = \sum_{j\neq k} \nabla_k \left(u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj}) \right) \tag{46}$$

Combining (I), (II), (III) and (IV), we we will get that the second derivative of the trial function is:

$$\begin{aligned} \frac{1}{\Psi_t} \nabla_k^2 \Psi_T = \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_{\phi(\mathbf{r}_k)})} + 2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \left(\sum_{j\neq k} \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} u'(r_{kj}) \right) + \\ \sum_{i,j\neq k} \left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) \left(\frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} \right) u'(r_{kj}) u'(r_{ki}) + \sum_{j\neq k} \nabla_k \left(u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj}) \right) \end{aligned} \tag{47}$$