FYS4411 - Computational quantum mechanics

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Project 1; Variational Monte Carlo Studies of Bosonic systems

temporary report

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Abstract

Some text that is abstact

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2.1.1 Simplified problem

The local energy is defined as:

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} H \Psi_T(\mathbf{R}), \tag{1}$$

As a first approximation, it is assumed there is no interaction term in the Hamiltonian, which means the hard sphere bosons have no physical size (the hard-core diameter is zero). It is also assumed that no magnetic field is applied to the bosonic gas, leaving a perfectly spherically symmetrical harmonic trap. Inserting this new Hamiltonian into the local energy gives:

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega_{ho}^2 r_i^2 \right) \Psi_T(\mathbf{R}) \tag{2}$$

The potential term is trivial since this is a scalar, i.e. the denominator will cancel the wavefunction. A more challenging problem is to find an expression for $\nabla_i^2 \Psi_T(\mathbf{R})$. The trial wavefunction shown in equation (...), with the aforementioned approximations, is:

$$\Psi_T(\mathbf{R}) = \prod_i e^{-\alpha r_i^2} \tag{3}$$

where α is the variational parameter for VCM. The first derivative is:

$$\begin{aligned} \nabla_j \prod_i e^{-\alpha r_i^2} &= -2\alpha \mathbf{r}_j e^{-\alpha r_j^2} \prod_{i \neq j} e^{-\alpha r_i^2} \qquad (4) \\ &= -2\alpha \mathbf{r}_j \prod_i e^{-\alpha r_i^2}. \qquad (5) \end{aligned}$$

The second derivative then follows:

$$\begin{aligned} \nabla_j^2 \prod_i e^{-\alpha r_i^2} &= \nabla_j \left(-2\alpha \mathbf{r}_j \prod_i e^{-\alpha r_i^2} \right) \qquad (6) \\ &= \left(4\alpha^2 r_j^2 - 2d\alpha \right) \prod_i e^{-\alpha r_i^2}. \qquad (7) \end{aligned}$$

where d is the number of dimensions. Inserting this into back into the local energy (equation (2)), the final expression can be derived:

$$\begin{aligned} E_L(\mathbf{R}) &= \frac{1}{\Psi_T(\mathbf{R})} \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega_{ho}^2 r^2 \right) \Psi_T(\mathbf{R}) \\ &= \sum_{i=1}^N \left[\frac{-\hbar^2}{2m} \left(4\alpha^2 r_i^2 - 2d\alpha \right) + \frac{1}{2} m \omega_{ho}^2 r_i^2 \right] \end{aligned}$$

The drift force (quantum force), still with the approximations above, is defined by:

$$F = \frac{2\nabla \Psi_T}{\Psi_T} \tag{8}$$

The gradient here is defined as

$$\nabla \equiv (\nabla_1, \nabla_2, \ldots, \nabla_N)$$

i.e. a vector of dimension Nd. The gradient with respect to a single particle's position is already given in equation 5, so it's not too hard to realise:

$$
\begin{aligned}
F &= \frac{-4\alpha}{\Psi_T}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right)\Psi_T \\
&= -4\alpha\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right)
\end{aligned}
$$

2.1.2 Full problem

The full local energy[1] is a bit more tedious to derive. The first step is to rewrite the trial wavefunction to the following form:

$$
\Psi_T(\mathbf{R}) = \prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \tag{9}
$$

where, in order for this to fit with the previous wavefunction, $u(r_{ij}) \equiv \ln[f(r_{ij})]$ and $\phi(\mathbf{r}_i) \equiv g(\alpha, \beta, \mathbf{r}_i)$. The gradient with respect to the k-th coordinate set is:

$$
\begin{aligned}
\nabla_k \Psi_T &= \nabla_k \prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} &(10)\\
&= \nabla_k \phi_k \left[\prod_{i\neq k} \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})}\right] + \left[\prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \nabla_k \left(\sum_{i''<j''} u_{i''j''}\right)\right] &(11)\\
&= \nabla_k \phi_k \left[\prod_{i\neq k} \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})}\right] + \left[\prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \left(\sum_{i''<j''} \nabla_k u_{i''j''}\right)\right] &(12)
\end{aligned}
$$

The function u_{ij} is symmetric under permutation $i \leftrightarrow j$, as one can see from the definitions of u_{ij} and $f(r_{ij})$. Therefore, the last sum above can have a different indexing: All terms without an index k, will give zero when taking the derivative ∇_k, so only $i = k$ or $j = k$ remains (remember $i \neq j$). Due to the symmetry of u_{ij}, one can simply always say $i = k$ and let j be the summation index:

$$
\nabla_k \Psi_T = \nabla_k \phi_k \left[\prod_{i\neq k} \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})}\right] + \left[\prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \left(\sum_{j''\neq k} \nabla_k u_{kj''}\right)\right] \tag{13}
$$

The second derivative now becomes (where ∇_k only acts on the first parenthesis to its right):

$$
\begin{aligned}
\nabla_k^2 \Psi_T = {}& (\nabla_k^2 \phi_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})}\right] + (\nabla_k \phi_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i) \nabla_k e^{\sum_{i'<j'} u(r_{i'j'})}\right] \\
&+ \left[\nabla_k \left(\prod_i (\phi(\mathbf{r}_i))\, e^{\sum_{i'<j'} u(r_{i'j'})}\right) \left(\sum_{j''\neq k} \nabla_k u_{kj''}\right)\right] \\
&+ \left[\prod_i \phi(\mathbf{r}_i) e^{\sum_{i'<j'} u(r_{i'j'})} \left(\sum_{j''\neq k} \nabla_k^2 u_{kj''}\right)\right]
\end{aligned}
$$

While a bit of a nuisance to read, the expression above is simply the product rule for $\nabla_k(\nabla_k \Psi_T)$. Written in terms of Ψ_T, the above can be a bit simplified[2]:

$$
\begin{aligned}
\nabla_k^2 \Psi_T = {}& (\nabla_k^2 \phi_k) \frac{\Psi_T}{\phi(\mathbf{r}_k)} + (\nabla_k \phi_k) \left[\prod_{i\neq k} \phi(\mathbf{r}_i) \nabla_k e^{\sum_{i'<j'} u(r_{i'j'})}\right] \\
&+ \left[(\nabla_k \Psi_T) \left(\sum_{j''\neq k} \nabla_k u_{kj''}\right)\right] \\
&+ \left[\Psi_T \left(\sum_{j''\neq k} \nabla_k^2 u_{kj''}\right)\right]
\end{aligned}
$$

[1] The "full local energy" means not making any assumptions on the particle interactions or the potential.

[2] For the more mathematically concerned nitpicker, the product symbol only runs over the functions $\phi(\mathbf{r}_i)$), not the following exponential. This is easy to realise by recalling how Ψ_T was defined, and is important to know when inserting Ψ_T as done now.

The second term above is equal to the second term in equation 13, divided by $\phi(\mathbf{r}_k)$. Furthermore, the gradient $\nabla_k \Psi_T$ is already calculated above, and in terms of Ψ_T is:

$$\nabla_k \Psi_T = \frac{\Psi_T}{\phi(\mathbf{r}_k)} \nabla_k \phi_k + \Psi_T \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \tag{14}$$

Inserting all this back into the second derivative yields:

$$\begin{aligned}
\nabla_k^2 \Psi_T = (\nabla_k^2 \phi_k) \frac{\Psi_T}{\phi(\mathbf{r}_k)} &+ (\nabla_k \phi_k) \left[\frac{\Psi_T}{\phi(\mathbf{r}_k)} \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \right] \\
&+ \left[\frac{\Psi_T}{\phi(\mathbf{r}_k)} \nabla_k \phi_k + \Psi_T \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \right] \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \\
&+ \left[\Psi_T \left(\sum_{j'' \neq k} \nabla_k^2 u_{kj''} \right) \right]
\end{aligned}$$

Giving:

$$\begin{aligned}
\frac{1}{\Psi_T} \nabla_k^2 \Psi_T = (\nabla_k^2 \phi_k) \frac{1}{\phi(\mathbf{r}_k)} &+ (\nabla_k \phi_k) \left[\frac{1}{\phi(\mathbf{r}_k)} \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \right] \\
&+ \left[\frac{1}{\phi(\mathbf{r}_k)} \nabla_k \phi_k + \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \right] \left(\sum_{j'' \neq k} \nabla_k u_{kj''} \right) \\
&+ \sum_{j'' \neq k} \nabla_k^2 u_{kj''}
\end{aligned}$$

Which can be rewritten to:

$$\frac{1}{\Psi_T} \nabla_k^2 \Psi_T = \frac{\nabla_k^2 \phi_k}{\phi(\mathbf{r}_k)} + \frac{2 \nabla_k \phi_k}{\phi(\mathbf{r}_k)} \left(\sum_{i \neq k} \nabla_k u_{ki} \right) + \left(\sum_{j \neq k} \nabla_k u_{kj} \right)^2 + \sum_{l \neq k} \nabla_k^2 u_{kl} \tag{15}$$

The gradients $\nabla_k u_{ki}$ can be rewritten using partial differentiation (where $r_{k,i}$ is coordinate i of $\mathbf{r}_k$):

$$\begin{aligned}
\nabla_k u_{ki} &= \left(\frac{\partial}{\partial r_{k,1}}, \frac{\partial}{\partial r_{k,2}}, \dots \right) u_{ki} \\
&= \frac{\partial u_{ki}}{\partial r_{ki}} \left(\frac{\partial r_{ki}}{\partial r_{k,1}}, \frac{\partial r_{ki}}{\partial r_{k,2}}, \dots \right) \\
&= \frac{\partial u_{ki}}{\partial r_{ki}} \left(\frac{\partial}{\partial r_{k,1}} \left(\sqrt{[(r_{k,1} - r_{i,1}) \hat{e}_1 + \dots]^2} \right), \dots \right) \\
&= \frac{\partial u_{ki}}{\partial r_{ki}} \left(\frac{r_{k,1} - r_{i,1}}{r_{ki}}, \dots \right) \\
&= \frac{\partial u_{ki}}{\partial r_{ki}} \frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} \\
&= \frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} u'_{ki} \ , \ \ u'_{ki} \equiv \frac{\partial u_{ki}}{\partial r_{ki}}
\end{aligned}$$

While the second derivative of u_{ki} is:

$$
\begin{aligned}
\nabla_k^2 u_{ki} &= \nabla_k(\nabla_k u_{ki}) \\
&= u'_{ki}\nabla_k\left(\frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}\right) + \frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}\nabla_k u'_{ki} \\
&= u'_{ki}\left(\frac{d}{r_{ki}} - \frac{r_{k,1}-r_{i,1}}{r_{ki}^3} - \frac{r_{k,2}-r_{i,2}}{r_{ki}^3} - \dots\right) + \frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}\cdot\frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}u''_{ki} \\
&= \frac{u'_{ki}}{r_{ki}}\left(d - \frac{r_{k,1}-r_{i,1}}{r_{ki}^2} - \frac{r_{k,2}-r_{i,2}}{r_{ki}^2} - \dots\right) + u_{ki} \\
&= \frac{u'_{ki}}{r_{ki}}(d-1) + u_{ki}
\end{aligned}
$$

where d, as earlier, is the number of dimensions present, which in our world is usually $d = 3$. Finally, this gives:

$$
\frac{1}{\Psi_T}\nabla_k^2\Psi_T = \frac{\nabla_k^2\phi_k}{\phi(\mathbf{r}_k)} + \frac{2\nabla_k\phi_k}{\phi(\mathbf{r}_k)}\left(\sum_{i\neq k}\frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}u'_{ki}\right) + \sum_{i,j\neq k}\frac{(\mathbf{r}_k-\mathbf{r}_i)(\mathbf{r}_k-\mathbf{r}_j)}{r_{ki}r_{kj}}u'_{ki}u'_{kj} + \sum_{l\neq k}u_{ki} + \frac{u'_{ki}}{r_{ki}}(d-1) \tag{16}
$$

As the exact forms of ϕ_k and u_{ki} are known, this can be written to a more recognisable, and calculable, expression. However, this expression will be quite long, so only the necessary variables will be derived. Inserting them into equation 16 is trivial. The u_{ki} derivatives are:

$$
\frac{\partial u_{ki}}{\partial r_{ki}} = \frac{\partial}{\partial r_{ki}}\left(\ln\left[1-\frac{a}{r_{ki}}\right]\right) = \frac{a}{r_{ij}^2 - ar_{ij}} \tag{17}
$$

$$
\frac{\partial^2 u_{ki}}{\partial r_{ki}^2} = \frac{\partial}{\partial r_{ki}}u'_{ki} = -a\frac{2r_{ki}-a}{r_{ki}^2 - ar_{ki}} \tag{18}
$$

and the ϕ_k derivatives are:

$$
\nabla_k\phi_k = \nabla_k e^{-\alpha(x_k^2+y_k^2+\beta z_k^2)} = -2\alpha(x_k, y_k, \beta z_k)\phi_k \tag{19}
$$

$$
\nabla_k^2\phi_k = \nabla_k(\nabla_k\phi_k) = \left[-2\alpha(2+\beta) + 4\alpha^2(x_k^2+y_k^2+\beta^2 z_k^2)\right]\phi_k \tag{20}
$$

3 Results

N	D	Analytical	Numerical	Variance	Time
1	1	0			
1	2	0			
1	3	0.88			
10	1				
10	2	10	10	7.4e-13	1.35
10	3	15	15	3.7e-13	1.41
100	1				
100	2				
100	3	150	150	8.5e-9	119.38
500	1				
500	2				
500	3	250	250	4.1e-8	316.19

Table 1: some caption

4 Conclusions

5 Appendix