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 Preliminary derivations

### 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 $\alpha$ is the variational parameter for VCM. The first derivative is:

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

The second derivative then follows:

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

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 $\nabla_k$, 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 $\nabla_k$ 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 $\Psi_T$, 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 $\Psi_T$ was defined, and is important to know when inserting $\Psi_T$ 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 $\Psi_T$ 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 $\mathbf{r}_k$):

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

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 $\phi_k$ 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 $\phi_k$ derivatives are:

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

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

## 2.2 The method of steepest descent

In order to find the value for $\alpha$ that minimizes $\langle E_L\rangle$, the method of steepest descent (SD) is applied. The SD method, in algorithm form, is:

$$
x_{n+1}=x_n-\gamma_n\nabla f \tag{21}
$$

where $x$ is the variable with which one wishes to find the minimum of $f$. In application to the current problem, $f=\langle E_L\rangle$. However, since $\langle E_L\rangle$ is an expensive quantity to find numerically, and its derivative ($\bar{E}_\alpha\equiv\frac{d\langle E_L\rangle}{d\alpha}$) even more so, an analytical expression is desirable. This can be found as follows:

$$
\begin{aligned}
\bar{E}_\alpha &= \frac{d}{d\alpha}\int dxP(x)E_L \\
&= \frac{d}{d\alpha}\int dx\frac{|\psi|^2}{\int dx'|\psi|^2}\frac{1}{\psi}H\psi \\
&= \frac{d}{d\alpha}\int dx\frac{\psi^*H\psi}{\int dx'|\psi|^2}
\end{aligned} \tag{22}
$$

Since the Hamiltonian is hermitian, one has $\int dx\psi^*H\psi=\int dxH\psi^*\psi$, giving:

$$
\begin{aligned}
&= \frac{d}{d\alpha}\int dx\frac{H\psi^*\psi}{\int dx'|\psi|^2} \\
&= \left[\int dx\frac{H\left(\psi^*\left(\frac{d\psi}{d\alpha}\right)+\left(\frac{d\psi^*}{d\alpha}\right)\psi\right)}{\int dx'|\psi|^2}\right]-\left[\int dx\frac{H\psi^*\psi}{\left(\int dx'|\psi|^2\right)^2}\int dx'\left(\psi^*\left(\frac{d\psi}{d\alpha}\right)+\left(\frac{d\psi^*}{d\alpha}\psi\right)\right)\right]
\end{aligned} \tag{23}
$$

Again one may use the hermiticity of the Hamiltonian to get $\int dx H\psi^* \left(\frac{d\psi}{d\alpha}\right) = \int dx H \left(\frac{d\psi^*}{d\alpha}\right)\psi$. So:

$$
\begin{aligned}
&= 2\left[\int dx \frac{H\psi^* \frac{d\psi}{d\alpha}}{\int dx' |\psi|^2}\right] - 2\left[\int dx \frac{H\psi^*\psi}{\left(\int dx'|\psi|^2\right)^2} \int dx' \psi^* \frac{d\psi}{d\alpha}\right] \\
&= 2\left[\int dx \frac{H\psi^* \frac{d\psi}{d\alpha}}{\int dx' |\psi|^2} - \int dx \frac{H\psi^*\psi}{\int dx'|\psi|^2} \int dx' \frac{1}{\int dx'|\psi|^2} \psi^* \frac{d\psi}{d\alpha}\right] \\
&= 2\left[\int dx \frac{\psi^*\left(\frac{E_L}{\psi}\frac{d\psi}{d\alpha}\right)\psi}{\int dx'|\psi|^2} - \int dx \frac{\psi^* E_L \psi}{\int dx'|\psi|^2} \int dx' \frac{\psi^*\left(\frac{1}{\psi}\frac{d\psi}{d\alpha}\right)\psi}{\int dx'|\psi|^2}\right] \\
&= 2\left(\langle \frac{\bar{\psi}_\alpha}{\psi} E_L\rangle - \langle \frac{\bar{\psi}_\alpha}{\psi}\rangle\langle E_L\rangle\right)
\end{aligned}
\tag{24}
$$

where $\bar{\psi}_\alpha \equiv \frac{d\psi}{d\alpha}$. This is a much better expression to use since one only need one Monte Carlo cycle to find $\bar{E}_\alpha$. Therefore, one Monte Carlo cycle will give one value for $\bar{E}_L$.
Since $\alpha$ will only have to be determined once, it is permissible to do so with greater accuracy. This means ... (explain about higher accuracy and divisions by 2)

# 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