Practical considerations

regarding the calculation of the local energy

$$E_L[R] \equiv \frac{H\,\psi_T[R]}{\psi_T[R]} = -\frac{\hbar^2}{2\,m}\sum_i \frac{\nabla_i{}^2\,\psi_T[R]}{\psi_T[R]} + V[R]$$

The $\psi_T[R]$ wave function is built as a product of many terms, both one body and 2 - body type, which we can write as

$$\psi_T[R] = \prod_k f_k[R] \qquad (1)$$

Notice that the index i runs over the number of particles, whilst the index k runs over the number of terms ($f_k[R]$) participating in the construction of the variational wave - function.

The kinetic term $\nabla_i{}^2$ operates on $\psi_T[R]$ in a manner that can be simplified if we notice that

$$\nabla_i\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right) = \frac{\nabla_i{}^2\,\psi_T[R]}{\psi_T[R]} - \left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right)\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right)$$

and therefore

$$\frac{\nabla_i^{\,2}\,\psi_T[R]}{\psi_T[R]} = \left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right)\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right) + \nabla_i\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right) \qquad (2)$$

The advantage of using this form is that the term $\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right)$

is greatly simplified :

$$\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right) = \frac{\nabla_i\,(\prod_k\;f_k[R]\,)}{\prod_k\;f_k[R]} = \sum_k \frac{\nabla_i\;f_k[R]}{f_k[R]}$$

ie, it is simply a sum of individual terms $\frac{\nabla_i\;f_k[R]}{f_k[R]}$.

The same is true for $\nabla_i\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right)$, the remaining term in (2) :

$$\nabla_i\left(\frac{\nabla_i\;\psi_T[R]}{\psi_T[R]}\right) = \nabla_i\left(\sum_k \frac{\nabla_i\;f_k[R]}{f_k[R]}\right) = \left(\sum_k \nabla_i\left(\frac{\nabla_i\;f_k[R]}{f_k[R]}\right)\right)$$

ie, again it reduces to only having to deal with

single terms $\frac{\nabla_i\;f_k[R]}{f_k[R]}$