Local Energy Gradient Derivation

$$\nabla_\alpha \langle E_L \rangle = \nabla_\alpha \langle H \rangle = \nabla_\alpha \left(\frac{\int d\mathrm{R} \Psi^* \mathcal{H} \Psi}{\int d\mathrm{R} |\Psi|^2} \right)$$

$$= \frac{\left(\int d\mathrm{R}|\Psi|^2\right)\nabla_\alpha\left(\int d\mathrm{R}\Psi^*\mathcal{H}\Psi\right) - \left(\int d\mathrm{R}\Psi^*\mathcal{H}\Psi\right)\nabla_\alpha\left(\int d\mathrm{R}|\Psi|^2\right)}{\left(\int d\mathrm{R}|\Psi|^2\right)^2}$$

$$= \frac{\int d\mathrm{R}\left[\nabla_\alpha\left(\Psi^*\right)\mathcal{H}\Psi + \Psi^*\nabla_\alpha(\mathcal{H}\Psi)\right]}{\int d\mathrm{R}|\Psi|^2} - \frac{\left(\int d\mathrm{R}\Psi^*\mathcal{H}\Psi\right)\int d\mathrm{R}\nabla_\alpha|\Psi|^2}{\left(\int d\mathrm{R}|\Psi|^2\right)^2}$$

$$= \frac{\int d\mathrm{R}|\Psi|^2 \frac{\nabla_\alpha\left(\Psi^*\right)\mathcal{H}\Psi + \Psi^*\nabla_\alpha(\mathcal{H}\Psi)}{|\Psi|^2}}{\int d\mathrm{R}|\Psi|^2} - \frac{\int d\mathrm{R}\Psi^*\mathcal{H}\Psi}{\int d\mathrm{R}|\Psi|^2}\frac{\int d\mathrm{R}|\Psi|^2\frac{\nabla_\alpha|\Psi|^2}{|\Psi|^2}}{\int d\mathrm{R}|\Psi|^2}$$

$$= \left\langle \frac{\nabla_\alpha\left(\Psi^*\right)\mathcal{H}\Psi + \Psi^*\nabla_\alpha(\mathcal{H}\Psi)}{|\Psi|^2} \right\rangle - \langle H \rangle \left\langle \frac{\nabla_\alpha|\Psi|^2}{|\Psi|^2} \right\rangle$$

$$= \left\langle \frac{\nabla_\alpha\left(\Psi^*\right)\mathcal{H}\Psi + \nabla_\alpha\left(\Psi^*\right)\mathcal{H}\Psi}{|\Psi|^2} \right\rangle - \langle H \rangle \left\langle \frac{2|\Psi|\nabla_\alpha|\Psi|}{|\Psi|^2} \right\rangle$$

$$= \left\langle \frac{2\nabla_\alpha\Psi^*}{\Psi^*}E_L \right\rangle - \langle E_L \rangle \left\langle \frac{2\nabla_\alpha|\Psi|}{|\Psi|} \right\rangle = 2\left[\left\langle \frac{\nabla_\alpha\Psi^*}{\Psi^*}E_L \right\rangle - \langle E_L \rangle \left\langle \frac{\nabla_\alpha|\Psi|}{|\Psi|} \right\rangle \right]$$

Depending on the trial function, in particular if the trial function is proportional to an exponential, the following equivalent expression might be easier to compute.

$$\nabla_\alpha \langle E_L \rangle = 2\left[\left\langle E_L \nabla_\alpha \ln \Psi^* \right\rangle - \langle E_L \rangle \langle \nabla_\alpha \ln|\Psi| \rangle \right]$$

Simple Gaussian trial function:

For $\Psi_T(\mathrm{R},\alpha) = \prod_i^N g(\mathrm{r}_i,\ \alpha)$ where $g(\mathrm{r}_i,\ \alpha) = \exp\left(-\alpha \mathrm{r}_i^2\right)$. We have $|\Psi_T| = \Psi_T^* = \Psi_T$ because the function is real and (strictly) positive.

$$\ln \Psi_T = \ln\left[\prod_i^N g(\mathrm{r}_i,\ \alpha)\right] = \sum_i^N \ln[g(\mathrm{r}_i,\alpha)] = \sum_i^N \ln\left[\exp\left(-\alpha \mathrm{r}_i^2\right)\right] = -\alpha\sum_i^N \mathrm{r}_i^2$$

$$\frac{\partial}{\partial\alpha}\ln\Psi_T = -\sum_i^N \mathrm{r}_i^2$$

We thus have

$$\frac{\partial}{\partial\alpha}\langle E_L\rangle = 2\left[\left\langle -\sum_i^N \mathrm{r}_i^2 E_L\right\rangle - \langle E_L\rangle\left\langle -\sum_i^N \mathrm{r}_i^2\right\rangle\right]$$

$$= 2\left[\langle E_L\rangle\left\langle \sum_i^N \mathrm{r}_i^2\right\rangle - \left\langle \sum_i^N \mathrm{r}_i^2 E_L\right\rangle\right]$$

Asshole trial function:

$$\Psi_T(\mathrm{R},\alpha,\beta) = \prod_i^N g(\mathrm{r}_i,\alpha,\beta)\prod_{j<k}^N f(r_{jk},a) \text{ where } g(\mathrm{r}_i,\alpha,\beta) = \exp\left[-\alpha\left(x_i^2+y_i^2+\beta z_i^2\right)\right]$$

and $f(r_{jk},a) = \begin{cases} 0 & r_{jk}\le a \\ 1-\dfrac{a}{r_{jk}} & r_{jk} > a \end{cases}$

We again have $|\Psi_T| = \Psi_T^* = \Psi_T$ because the function is real and positive.

Using the gradient expression with fractions (as opposed to natural logs) is probably (a lot) more computationally efficient for this trial function.

$$\frac{\partial}{\partial\alpha}\Psi_T \propto \frac{\partial}{\partial\alpha}\prod_i^N g(\mathrm{r}_i,\alpha,\beta)$$

$$= \sum_l^N \left[\frac{\partial}{\partial\alpha} g(\mathrm{r}_l,\alpha,\beta)\right]\prod_{i\neq l}^N g(\mathrm{r}_i,\alpha,\beta) = -\sum_l^N \left(x_l^2+y_l^2+\beta z_l^2\right) g(\mathrm{r}_l,\alpha,\beta)\prod_{i\neq l}^N g(\mathrm{r}_i,\alpha,\beta)$$

$$= -\sum_l^N \left(x_l^2+y_l^2+\beta z_l^2\right)\prod_i^N g(\mathrm{r}_i,\alpha,\beta) = -\prod_i^N g(\mathrm{r}_i,\alpha,\beta)\sum_l^N \left(x_l^2+y_l^2+\beta z_l^2\right)$$

$$\frac{\partial}{\partial\alpha}\Psi_T = -\prod_i^N g(\mathrm{r}_i,\alpha,\beta)\prod_{j<k}^N f(r_{jk},a)\sum_l^N \left(x_l^2+y_l^2+\beta z_l^2\right) = -\Psi_T\sum_l^N \left(x_l^2+y_l^2+\beta z_l^2\right)$$

$$\frac{\partial_\alpha \Psi_T}{\Psi_T} = -\sum_l^N \left(x_l^2+y_l^2+\beta z_l^2\right)$$

Similarly we have

$$\frac{\partial}{\partial\beta}\Psi_T \propto \sum_l^N \left[\frac{\partial}{\partial\beta} g(\mathrm{r}_l,\alpha,\beta)\right]\prod_{i\neq l}^N g(\mathrm{r}_i,\alpha,\beta)$$

$$= -\sum_l^N \alpha z_l^2 g(\mathrm{r}_l,\alpha,\beta)\prod_{i\neq l}^N g(\mathrm{r}_i,\alpha,\beta) = -\prod_i^N g(\mathrm{r}_i,\alpha,\beta)\alpha\sum_l^N z_l^2$$

$$\frac{\partial}{\partial\beta}\Psi_T = -\prod_i^N g(\mathrm{r}_i,\alpha,\beta)\prod_{j<k}^N f(r_{jk},a)\alpha\sum_l^N z_l^2 = -\Psi_T\alpha^N\sum_l^N z_l^2$$

$$\frac{\partial_\beta \Psi_T}{\Psi_T} = -\alpha^N \sum_l^N z_l^2$$

Putting everything together;

$$\frac{\partial}{\partial\alpha}\langle E_L\rangle = 2\left[\left\langle \frac{\partial_\alpha \Psi_T}{\Psi_T} E_L \right\rangle - \langle E_L\rangle \left\langle \frac{\partial_\alpha \Psi_T}{\Psi_T} \right\rangle\right]$$

$$= 2\left[\left\langle -\sum_l^N \left(x_l^2 + y_l^2 + \beta z_l^2\right) E_L \right\rangle - \langle E_L\rangle \left\langle -\sum_l^N \left(x_l^2 + y_l^2 + \beta z_l^2\right) \right\rangle\right]$$

$$= 2\left[\langle E_L\rangle \left\langle \sum_l^N \left(x_l^2 + y_l^2 + \beta z_l^2\right) \right\rangle - \left\langle E_L \sum_l^N \left(x_l^2 + y_l^2 + \beta z_l^2\right) \right\rangle\right]$$

$$\frac{\partial}{\partial\beta}\langle E_L\rangle = 2\left[\left\langle \frac{\partial_\beta \Psi_T}{\Psi_T} E_L \right\rangle - \langle E_L\rangle \left\langle \frac{\partial_\beta \Psi_T}{\Psi_T} \right\rangle\right]$$

$$= 2\left[\left\langle -\alpha^N \sum_l^N z_l^2 E_L \right\rangle - \langle E_L\rangle \left\langle -\alpha^N \sum_l^N z_l^2 \right\rangle\right] = 2\alpha^N \left[\langle E_L\rangle \left\langle \sum_l^N z_l^2 \right\rangle - \left\langle E_L \sum_l^N z_l^2 \right\rangle\right]$$