Local Energy Gradient Derivation

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

$$= \frac{\left(\int d\mathbf{R}|\Psi|^2\right)\boldsymbol{\nabla}_{\boldsymbol{\alpha}}\left(\int d\mathbf{R}\Psi^*\mathcal{H}\Psi\right) - \left(\int d\mathbf{R}\Psi^*\mathcal{H}\Psi\right)\boldsymbol{\nabla}_{\boldsymbol{\alpha}}\left(\int d\mathbf{R}|\Psi|^2\right)}{\left(\int d\mathbf{R}|\Psi|^2\right)^2}$$

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

$$= \frac{\int d\mathbf{R}|\Psi|^2\frac{\boldsymbol{\nabla}_{\boldsymbol{\alpha}}\left(\Psi^*\right)\mathcal{H}\Psi + \Psi^*\boldsymbol{\nabla}_{\boldsymbol{\alpha}}(\mathcal{H}\Psi)}{|\Psi|^2}}{\int d\mathbf{R}|\Psi|^2} - \frac{\int d\mathbf{R}\Psi^*\mathcal{H}\Psi}{\int d\mathbf{R}|\Psi|^2}\frac{\int d\mathbf{R}|\Psi|^2\frac{\boldsymbol{\nabla}_{\boldsymbol{\alpha}}|\Psi|^2}{|\Psi|^2}}{\int d\mathbf{R}|\Psi|^2}$$

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

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

$$= \left\langle\frac{2\boldsymbol{\nabla}_{\boldsymbol{\alpha}}\left(\Psi^*\right)}{\Psi^*}E_L\right\rangle - \langle E_L\rangle\left\langle\frac{2\boldsymbol{\nabla}_{\boldsymbol{\alpha}}|\Psi|}{|\Psi|}\right\rangle = 2\left(\left\langle\frac{\boldsymbol{\nabla}_{\boldsymbol{\alpha}}\left(\Psi^*\right)}{\Psi^*}E_L\right\rangle - \langle E_L\rangle\left\langle\frac{\boldsymbol{\nabla}_{\boldsymbol{\alpha}}|\Psi|}{|\Psi|}\right\rangle\right)$$