

$$E_L(\mathbf{R}; \alpha) = \frac{1}{\Psi(\mathbf{R}; \alpha)} H \Psi(\mathbf{R}; \alpha) = \frac{1}{\Psi(\mathbf{R}; \alpha)} \left[ -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{R}; \alpha) + V(\mathbf{R}) \Psi(\mathbf{R}; \alpha) \right]$$

$$\text{where } \nabla^2 = \sum_i^N \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}$$

$$\text{We approximate } \frac{\partial^2 \Psi(x_i; \alpha)}{\partial x_i^2} \approx \frac{\Psi(x_i + h) - 2\Psi(x_i) + \Psi(x_i - h)}{h^2}$$

$$\nabla^2 \Psi_T(\mathbf{R}) = \sum_i^N \frac{\partial^2 \Psi_T}{\partial x_i^2} + \frac{\partial^2 \Psi_T}{\partial y_i^2} + \frac{\partial^2 \Psi_T}{\partial z_i^2}$$

$$\text{If the wavefunction is separable: } \Psi_T(\mathbf{R}) = \prod_j^N \psi_j(\mathbf{r}_j) \text{ then}$$

$$\frac{\partial^2 \Psi_T}{\partial x_i^2} = \frac{1}{\psi_i(\mathbf{r}_i)} \frac{\partial^2 \psi_i(\mathbf{r}_i)}{\partial x_i^2} \prod_j^N \psi_j(\mathbf{r}_j) = \frac{1}{\psi_i(\mathbf{r}_i)} \frac{\partial^2 \psi_i(\mathbf{r}_i)}{\partial x_i^2} \Psi_T(\mathbf{R})$$

$$\nabla^2 \Psi_T(\mathbf{R}) = \Psi_T(\mathbf{R}) \sum_i^N \frac{1}{\psi_i(\mathbf{r}_i)} \left[ \frac{\partial^2 \psi_i(\mathbf{r}_i)}{\partial x_i^2} + \frac{\partial^2 \psi_i(\mathbf{r}_i)}{\partial y_i^2} + \frac{\partial^2 \psi_i(\mathbf{r}_i)}{\partial z_i^2} \right]$$

$$\begin{aligned} &\approx \Psi_T(\mathbf{R}) \sum_i^N \frac{1}{\psi_i(\mathbf{r}_i) h^2} \{ \psi_i(x_i + h) + \psi_i(y_i + h) + \psi_i(z_i + h) + \psi_i(x_i - h) + \psi_i(y_i - h) + \psi_i(z_i - h) - 6\psi_i(\mathbf{r}_i) \} \\ &= \Psi_T(\mathbf{R}) \frac{1}{h^2} \sum_i^N \left\{ \frac{\psi_i(x_i + h) + \psi_i(y_i + h) + \psi_i(z_i + h) + \psi_i(x_i - h) + \psi_i(y_i - h) + \psi_i(z_i - h)}{\psi_i(\mathbf{r}_i)} - 6 \right\} \end{aligned}$$

Thus the kinetic energy contribution to the local energy is

$$-\frac{\hbar^2}{2m} \cdot \frac{1}{h^2} \sum_i^N \left\{ \frac{\psi_i(x_i + h) + \psi_i(y_i + h) + \psi_i(z_i + h) + \psi_i(x_i - h) + \psi_i(y_i - h) + \psi_i(z_i - h)}{\psi_i(\mathbf{r}_i)} - 6 \right\}$$