

The $H_{kk'}$ matrix elements are

$$K_{kk'} = -\frac{\hbar^2}{m} \int_0^\infty \phi_k(r) \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) \phi_{k'}(r) r^2 dr$$

$$V_{kk'} = \int_0^\infty \phi_k(r) V(r) \phi_{k'}(r) r^2 dr$$

In general :

* $K_{kk'}$ are analytical

* $V_{kk'} \rightarrow \approx N^2/2$ integrals with high accuracy (10^{-7})

Let us introduce a Gaussian quadrature

$$V_{kk'} \approx \sum_{\alpha=0}^{N-1} w_\alpha \phi_k(x_\alpha) V(x_\alpha) \phi_{k'}(x_\alpha)$$

with $\{x_\alpha\}; \{w_\alpha\}$ ($\alpha=0, 1, \dots, N-1$) are the Gaussian weights and points