

Need for calculation of coupled wave functions

Coupled channel bound states calculations for alkali dimers using the Fourier grid method

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$$\mathbf{H}\psi = (\mathbf{T} + \mathbf{V})\psi = E\psi.$$

$$\mathbf{V}_{ij} = V(R_i) \delta_{ij}.$$

$$T_{ii} = \frac{\hbar^2}{4\mu L^2} \frac{N^2 + 2}{6},$$

$$T_{ij} = (-1)^{i-j} \frac{\hbar^2}{4\mu L^2} \frac{1}{\sin^2[(i-j)\pi/N]} \quad \text{for } i \neq j.$$

$$\begin{pmatrix} \mathbf{H}_{AA} & \mathbf{H}_{AB} \\ \mathbf{H}_{BA} & \mathbf{H}_{BB} \end{pmatrix} = \begin{pmatrix} \mathbf{T} & \mathbf{0} \\ \mathbf{0} & \mathbf{T} \end{pmatrix} + \begin{pmatrix} \mathbf{V}_A & \mathbf{V}_{AB} \\ \mathbf{V}_{AB} & \mathbf{V}_B \end{pmatrix},$$

+ Variable step size

