One-dimensional double-well quantum oscillator

To expand the eigenstates of a double-well system with Hamiltonian:

$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2\left[\frac{(x^2-x_0^2)^2}{4x_0^2} - x^2\right],$$

we take the eigenstates of the normal harmonic oscillator as basis functions, i.e.

$$\psi_m(x) = \sum_n C_{mn}\,\phi_n(x),$$

where $\phi_n(x)$ are the eigenstates of the quantum harmonic oscillator,

$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2.$$

The analytical form of $\phi_n(x)$ is known as:

$$\phi_n(x) = \left(\frac{m\omega_0}{\hbar}\right)^{1/4}\frac{1}{\left[2^n\, n!\,\sqrt{\pi}\right]^{1/2}} H_n(\xi)\, e^{-\xi^2/2},$$

where $H_n(\xi)$ is the Hermite Polynormials. $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$

A few lowest-order terms are:

$$\mathcal{H}_0 = 1,\ \mathcal{H}_1 = 2\xi,\ \mathcal{H}_2 = -2 + 4\xi^2,\ \mathcal{H}_3 = -12\xi + 8\xi^3,\ \cdots$$

To numerically represent $\phi_n(x)$ seems to be very challenging due to the presence of $n!$, which becomes straightforward after adopting the recursive relation:

$$\mathcal{H}_{n+1}(\xi) = 2\xi\,\mathcal{H}_n(\xi) - 2n\,\mathcal{H}_{n-1}(\xi),$$

$$\mathcal{H}_n'(\xi) = 2n\,\mathcal{H}_{n-1}(\xi).$$

Based on it, a recursive relation for $\phi_n(x)$ can be easily obtained.

$$\phi_n(x) = \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{4}} \frac{1}{[2^n n!\sqrt{\pi}]^{\frac{1}{2}}} \mathcal{H}_n(\xi)\, e^{-\frac{\xi^2}{2}}$$

$$= \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{4}} \frac{1}{[2^n n!\sqrt{\pi}]^{\frac{1}{2}}} \left[2\xi\,\mathcal{H}_{n-1}(\xi) - 2(n-1)\mathcal{H}_{n-2}(\xi)\right] e^{-\xi^2/2}$$

$$= \frac{2\xi}{\sqrt{2n}}\phi_{n-1}(x) - \sqrt{\frac{n-1}{n}}\,\phi_{n-2}(x)$$