

Some title

The time independent Schrödinger equation for the harmonic oscillator is

$$-\frac{\hbar}{2m} \frac{d^2 u}{dx^2} + \frac{m\omega^2}{2} x^2 = Eu \quad (1)$$

By changing the variables with $\xi = x/\sqrt{\hbar/m\omega}$ and $E' = \hbar\omega$, it can be written as

$$-\frac{d^2 u}{d\xi^2} + \xi^2 u = 2E' u \quad (2)$$

Numerical solution to eigenvalue problem

We wish to solve (2) numerically by discretizing the real line and the second derivative of u . In order to do so, we introduce the gridpoints ξ_j and the approximation of the function u at these gridpoints, $u_j \approx u(\xi_j)$. Furthermore, we assume that $\xi_j \in [-L, L]$, where L is chosen such that $u(\xi) \approx 0$ for $|\xi| > L$. Since the eigenfunctions of an even potential can be taken to be even or odd, we can focus on the interval $[0, L]$ and apply the boundary conditions

$$\begin{aligned} u'(0) = 0 \quad \text{and} \quad u(L) = 0 \quad \text{for even } u, \\ u(0) = 0 \quad \text{and} \quad u(L) = 0 \quad \text{for odd } u. \end{aligned} \quad (3)$$

The second derivative is approximated up to fourth order:

$$\begin{aligned} u''(x_j) \approx \frac{1}{12h^2} (& -u_{j-2} + 16u_{j-1} - 30u_j \\ & + 16u_{j+1} - u_{j+2}) \end{aligned} \quad (4)$$

Special care had to be taken at the boundaries. For the even case, two ghost points, ξ_{-1} and ξ_{-2} , were introduced to the left of zero and two fourth order approximations of the first derivative used to (... words ...):

$$\begin{aligned} u'(0) &\approx \frac{1}{12h} (u_{-2} - 8u_{-1} + 8u_1 - u_2) \\ u'(0) &\approx \frac{1}{12h} (-3u_{-1} - 10u_0 + 18u_1 - 6u_2 + u_3) \end{aligned} \quad (5)$$