04 Aug '23

(c) Time - independent Schrodinger Eq for SHO -

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_j}{dx^2} + \frac{1}{2}m\omega^2 x^2 \varphi_j = E_j \varphi_j$$

The corresponding dimensionless equation is, (making the 1st term dimensionless will automatically make all terms dimensionless)

Define $\hat{x} = x/a$,

$$-\frac{\hbar^2}{2ma^2}\frac{d^2\varphi}{d\hat{x}^2} + \frac{1}{2}m\omega^2 \hat{x}^2 a^2 \varphi_j = E_j \varphi_j$$

$$\Rightarrow \quad -\frac{d^2\varphi}{d\hat{x}^2} + \frac{m^2\omega^2 a^4}{\hbar^2}\hat{x}^2\varphi_j = \frac{2ma^2 E_j}{\hbar^2}\varphi_j$$

Hence, $a^2 = \hbar/m\omega$ and $\hat{E} = 2E/\hbar\omega$,

$$-\frac{d^2\varphi_j}{d\hat{x}^2} + \hat{x}^2\varphi_j = \hat{E}\varphi_j$$

* BC : Dirichlet's $\{\varphi(-L) = \varphi(L) = 0$

Hence a central difference scheme on 2nd order derivative is apt.

$$-\left[\frac{1}{\Delta\hat{x}}\left(\frac{\varphi_j^{(n+1)} - \varphi_j^{(n)}}{\Delta\hat{x}} - \frac{\varphi_j^{(n)} - \varphi_j^{(n-1)}}{\Delta\hat{x}}\right)\right] + \hat{x}^2\varphi_j^{(n)} = \hat{E}_j\varphi_j^{(n)}$$

In Block matrix notation,

$$\frac{-1}{\Delta\hat{x}^2}\begin{bmatrix}1 & -2 & 1\end{bmatrix}\begin{bmatrix}\varphi_j^{(n-1)}\\ \varphi_j^{(n)}\\ \varphi_j^{(n+1)}\end{bmatrix} + \begin{bmatrix}0 & \hat{x}^2(n) & 0\end{bmatrix}\begin{bmatrix}\varphi_j^{(n-1)}\\ \varphi_j^{(n)}\\ \varphi_j^{(n+1)}\end{bmatrix} = \hat{E}_j\begin{bmatrix}\varphi_j^{(n-1)}\\ \varphi_j^{(n)}\\ \varphi_j^{(n+1)}\end{bmatrix}$$

Matrix Form (Incorporating BCs - $\varphi_j^{(0)} = \varphi_j^{(N+1)} = 0$)

$$\frac{-1}{\Delta\hat{x}^2}\begin{bmatrix}-2 & 1 & & & 0\\ 1 & -2 & 1 & \ddots & \\ & & 1 & -2 & 1 \\ & 0 & & \ddots & \\ & & & 1 & -2\end{bmatrix}\begin{bmatrix}\varphi_j^{(1)}\\ \varphi_j^{(2)}\\ \vdots\\ \varphi_j^{(n)}\\ \vdots\\ \varphi_j^{(N)}\end{bmatrix} + \begin{bmatrix}V_1 & & & 0\\ & V_2 & \ddots & \\ & & V_4 \ddots & \\ 0 & & & V_{N+1}\end{bmatrix}\begin{bmatrix}\varphi_j^{(1)}\\ \varphi_j^{(2)}\\ \vdots\\ \varphi_j^{(n)}\\ \vdots\\ \varphi_j^{(N)}\end{bmatrix} = \hat{E}_j\begin{bmatrix}\varphi_j^{(1)}\\ \varphi_j^{(2)}\\ \vdots\\ \varphi_j^{(n)}\\ \vdots\\ \varphi_j^{(N)}\end{bmatrix}$$

where $V_n = \hat{x}^2(n)$ ← normalized HO potential

$\hat{x} = x/\sqrt{\hbar/m\omega}$; $\hat{E} = 2E/\hbar\omega$

(ii) <u>Implementation</u> :

- A SHIFTED INVERSE POWER routine is used to find the 1st few eigen states and eigen values.

instead of calculating $A^{-1}x$, $Ay = x$ is solved for y, this is because :
- Numerically more stable and robust
- compactible with tridiagonal spare matrix optimizati

- Gauss elimination, Backsubstitution is used to solve $Ay = x$ mainly because of ease of implementation and compactibility with tridiagonal optimization.

- Trapezoid integration is implement for normalizing the wavefunctions for above reasons.

(iii) <u>Discussion</u> :

Quantum confinement and the associated increase in energy levels may be visualized in the gif provided.

- Ground and other state E levels increases with increasing confinement as seen from the normalized energy eigenvalues.

- The output is tested by using the scipy.special. Hermit polynomial module, where the confined HO is shown to converge in SHO both qualitatively (graphs in the GIF) and quantitatively (eigenvalues in GIF match that of known SHO eigen values, $E = (n+\frac{1}{2})\hbar\omega$ or in normalized $\tilde{E} = 2n+1$) as L becomes large.