Solutions to Schödringer Equation Visualized

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Erwin Schrödinger

- Ushered in paradigm shift in physics, published in 1926
- Solve for ψ

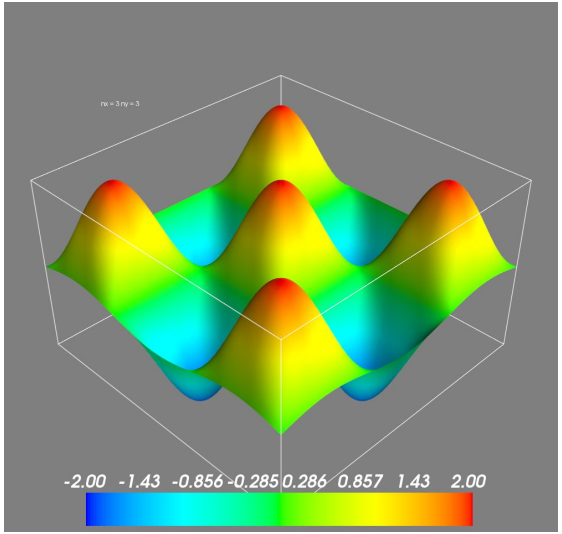
$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx} + U(x)\psi = E\psi$$

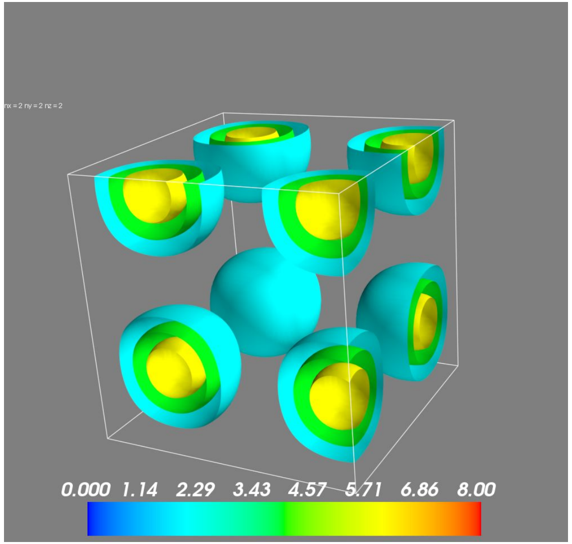
$$\frac{-\hbar^2}{2m}\Delta^2\Psi + U(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z)$$

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

Particle in a Box

Given a square potential, solutions 2D (or 3D) have the appearance of:

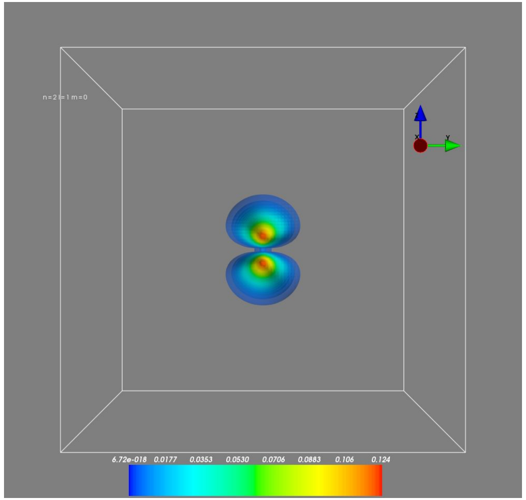




$$\Psi(x,y,z,t) = \sqrt{\frac{8}{L_x L_y L_z}} sin(k_x x) sin(k_y y) sin(k_z z) e^{-i\omega t}.$$

Radial Schrödinger Equation

- Equation can be converted to angular and radial coords



$$\psi(r,\theta,\phi) = \underbrace{R(r)}_{\text{Radial}}\,\underbrace{P(\theta)}_{\text{Polar}}\,\underbrace{F(\phi)}_{\text{Azimuth}}$$

$$\psi_{nlm}(r,\theta,\phi) = \sqrt{\frac{\rho^3}{r}\frac{(n-l-1)!}{2n(n+l)!}}\,e^{-\rho/2}\rho^l L^{2l+1}_{n-l-1}(\rho)Y_l^m(\theta,\phi)$$

Technology Used

- Python
- Mayavi
- Scipy
- Numpy