PHY202 – Quantum Mechanics

Summary of Topic 10: The Schrödinger Eq. in 3 dim

The Schrödinger Eq. in 3 dim

The Schrödinger Eq. can be easily generalized to 3 dimensions:

- The kinetic energy becomes,

$$\frac{p^2}{2m} = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right)$$

- the TISE becomes

$$\boxed{\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x,y,z)\right]\psi(x,y,z) = E\psi(x,y,z)}$$

- when $V(x,y,z) = V_x(x) + V_y(y) + V_z(z)$, the S. eq. for $\psi(x,y,z)$ can be split into three 1 dim. S. eqs. for x, y and z
  - the total wavefn $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$
  - the total energy $E = E_x + E_y + E_z$
- there may be more than one quantum state with the same value of the total energy E. This is called degeneracy.

The two-dimensional IPW

Consider a two dimensional square infinite potential well given by

$$V(x) = \begin{cases} 0 & 0 < x < L_x \text{ and } 0 < y < L_y \\ \infty & \text{otherwise.} \end{cases}$$

- The TISE now reads

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y) = E\psi(x,y)$$

  with the boundary conditions that $\psi(x,y) = 0$ at the four boundaries.

  In going from 3 to 2 dim's we've "cropped" the z-dependent part of the TISE.

- The solutions are

$$\psi_{nm}(x,y) = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right)\sqrt{\frac{2}{L_y}}\sin\left(\frac{m\pi}{L_y}y\right)$$

  where $n, m = 1, 2, 3, \ldots$ are the respective quantum numbers for the x and y directions.

- The total energy levels are $E_{nm} = \frac{n^2\hbar^2\pi^2}{2mL_x^2} + \frac{m^2\hbar^2\pi^2}{2mL_y^2}$

The 2-dim IPW and degeneracy

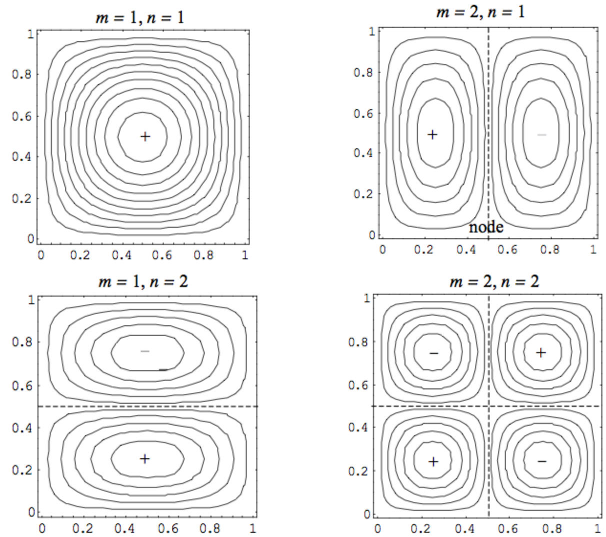
- When the IPW is square ($L_x = L_x = L$), then

$$E_{nm} = \frac{\hbar^2 \pi^2}{2mL^2} \left(n^2 + m^2\right)$$

- Since $E_{nm} = E_{mn}$, there is a two-fold degeneracy in the energy levels if $n \neq m$.

state (n, m)	$n^2 + m^2$	degeneracy
$(1,1)$	1	1
$(1,2)$, $(2,1)$	5	2
$(2,2)$	8	1
$(1,3)$, $(3,1)$	10	2

contour plots of $\psi_{nm}(x/L, y/L)$



- The degeneracy of the energy levels when $n \neq m$ is a consequence of the symmetry of the system. In this case it is the $x \leftrightarrow y$ invariance.

Further reading:
See, e.g., Phillips, pages 121-123.