

## L35-3d Hilbert Space and Hamiltonians

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\* Review solution of TDSE: (PDE)

$$\hat{H} \Psi(x,t) = \hat{E} \Psi(x,t) \quad \text{where } \hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}, \quad \hat{E} = i\hbar \partial_t$$

+ separation of variables:  $\Psi(x,t) = \psi(x) \phi(t)$

separate  $x$  on left,  $t$  on right, both equal constant  $E$ , leading to LHS, RHS eigenvalue equations

$$\begin{aligned} \hat{H} \psi(x) &= E \psi(x) & i\hbar \partial_t \phi(t) &= E \phi(t) \\ [\text{TISE}] \quad \text{eigenfunction} && \text{eigenfunction} &= e^{-iEt/\hbar} \end{aligned}$$

+ general solution is a linear combination of "tensor product" of building block eigenfunctions:

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iEt/\hbar} \quad \text{"skipping rope fns"}$$

+ coefficients (components) determined from initial conditions  $\Psi(x,0)$  and inner product,

$$\langle \psi_n | \Psi_0 \rangle = \sum_n c_n \underbrace{\langle \psi_n | \psi_n' \rangle}_{\delta_{nn'}} e^{-iE_n t/\hbar} = c_n$$

$$|\Psi(x,t)\rangle = \underbrace{\sum_n |\psi_n\rangle e^{-iE_n t/\hbar}}_{U(t)} \langle \psi_n | \Psi_0 \rangle = U(0,t) |\Psi_0\rangle = e^{-i\hat{H}t/\hbar} |\Psi_0\rangle$$

\* this same technique generalizes to 3-d:

+ 3-d wave functions:  $\Psi(\vec{r}) = \psi(x,y,z)$  or  $\Psi(r,\theta,\phi)$

norm:  $\int d\vec{r} |\Psi(\vec{r})|^2 = 1 \quad d\vec{r} = dx dy dz = r^2 \sin\theta d\theta d\phi dz.$

+ 3-d Schrödinger equation:

$$V(x) \rightarrow V(x, y, z) = V(\vec{r})$$

"Laplacian"  $\nabla^2$

$$\hat{T} = \frac{\hat{p}^2}{2m} \rightarrow \frac{\hat{p}^2}{2m} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} = \frac{-\hbar^2}{2m} (\partial_x^2 + \partial_y^2 + \partial_z^2) = -\frac{\hbar^2 \nabla^2}{2m}$$

+ Separation of Variables:  $\Psi(\vec{r}, t) = \psi(\vec{r}) \phi(t)$ ,  $\psi(\vec{r}) = X(x) Y(y) Z(z)$

• use eigenfunctions to substitute each operator with its eigenvalue

\* Example: 2-d infinite square well:  $0 < x < L$ ,  $0 < y < L$

$$-\frac{\hbar^2}{2m} \left( \underbrace{\partial_x^2}_{-k_x^2} + \underbrace{\partial_y^2}_{-k_y^2} \right) X(x) Y(y) \phi(t) = \underbrace{i\hbar \frac{d}{dt}}_{E=\hbar\omega} X(x) Y(y) \phi(t)$$

$$\partial_x^2 \sin(k_x x) = -k_x^2 \sin(k_x x) \text{ or } \cos(k_x x)$$

$$\partial_y^2 \sin(k_y y) = -k_y^2 \sin(k_y y) \text{ or } \cos(k_y y)$$

$$\partial_t e^{i\omega t} = i\omega e^{i\omega t}$$

$$\frac{\hbar^2}{2m} (k_x^2 + k_y^2) = \hbar\omega = E$$

- each spatial equation is a Sturm-Liouville system with boundary conditions

- apply B.C.'s separately in each dimension to get one quantum # per dimension:  $n, m$  for  $x, y$ .

+ Group activity: quantize  $k_x$  and  $k_y$  to obtain the energy spectrum  $E_{nm}$   
plot the node lines for each mode  $X_n(x) Y_m(y)$

+ Summary & application: Wien's law  $u(v) = \frac{8\pi v^3}{C^3} kT$

$$\# \text{ modes} = d_n^3 = n^2 dn ds = \left(\frac{2L}{C}\right)^3 v^2 dv \frac{4\pi}{8}$$

density of states  $g(v) = \frac{dN}{dv \cdot L^3} = \frac{8\pi v^2}{C^3}$

spectral intensity  $u(v) = g(v) \bar{\epsilon} = \frac{8\pi v^2}{C^3} kT$