

L33-3d 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" ∇^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 $g(\nu) = \frac{d^3n}{d\nu \cdot L^3} = \frac{8\pi\nu^2}{C^3}$

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