L27-3d Hilbert Space and Hamiltonians

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* Review solution of TDSE: (PDE)

$$\hat{H}\,\Psi(x,t) = \hat{E}\,\Psi(x,t) \quad \text{where } \hat{H}(x),\ \hat{E}(t),\ \Psi(x,t) = \psi(x)\,\phi(t)$$

- separation of variables: $= E\,\psi(x)\,\phi(t) \Rightarrow$ 2 ODE's

$$\Rightarrow \hat{H}\,\psi(x) = E\,\psi(x) \qquad \hat{E}\,\phi(t) = E\,\phi(t)$$

[TISE] $\qquad i\hbar\partial_t\,\underbrace{\phi(t)}_{\text{eigenfunction}} = E\,\phi(t) \qquad \phi(t) = e^{-iEt/\hbar}$

- general solution is a linear combination of "tensor product" of building blocks:

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

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

$$\langle\psi_n|\Psi_0\rangle = \sum_{n'} c_{n'}\,\underbrace{\langle\psi_n|\psi_{n'}\rangle}_{\delta_{nn'}}\,\cancelto{1}{e^{-iE_n 0/\hbar}} = c_n$$

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

* this same technique generalizes to 3-d:

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

norm: $\int d^3r\,|\psi(\vec{r})|^2 = 1 \qquad d^3r = dx\,dy\,dz = r^2\sin\theta\,d\theta\,d\phi\,dz.$

3-d Schrödinger equation:

$V(x) \to V(x,y,z) = V(\vec{r})$ "Laplacian"

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

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

- use eigenfunctions to substitute each operator with its eigenvalue

* Example: 2-d infinite square well:

$$\frac{-\hbar^2}{2m}\Big(\underbrace{\partial_x^2}_{-k_x^2} + \underbrace{\partial_y^2}_{-k_y^2}\Big) X(x)\,Y(y)\,\phi(t) = \underbrace{i\hbar\frac{\partial}{\partial t}}_{E} X(x)\,Y(y)\,\phi(t)$$

$\partial_x^2 \sin(k_x x) = -k_x^2 \sin(k_x x)$ or $\cos(k_x x)$ $\quad \partial_t e^{i\omega t} = i\omega\, e^{i\omega t}$

$\partial_y^2 \sin(k_y y) = -k_y^2 \sin(k_y y)$ $\quad \frac{\hbar^2}{2m}(k_x^2 + k_y^2) = \hbar\omega = E$

- 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 energy spectrum E_{nm}
plot the node lines for each mode $X_n(x)\,Y_m$

* Summary & application: Wien's law $u(\nu) = \frac{8\pi\nu^2}{c^3} kT$

$\#\text{modes} = d^3 n = n^2 dn\, d\Omega = \left(\frac{2L}{c}\right)^3 \nu^2 d\nu\; \frac{4\pi}{8}$

density of states $g(\nu) = \frac{dn}{d\nu \cdot L^3} = \frac{8\pi\nu^2}{c^3}$

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

* Application to central potentials:

$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(r)$ use spherical co-ords.

$$= \frac{\hbar^2}{2m}\cdot\frac{1}{r^2}\left[-\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \underbrace{\frac{-1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\left(\underbrace{\frac{\partial^2}{\partial\phi^2}}_{-m^2}\right)\right)}_{l(l+1)}\right] + V(r)$$

$$= \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2I}$$

- note: each equation is a Sturm-Liouville system:

$$\left[\frac{-1}{\omega}(D\,p\,D + q)\right] u_i(x) = \lambda_i u_i(x)$$

- azimuthal: $L_z \Phi(\phi) = -i\hbar\partial_\phi \left[e^{im\phi}\right] = \hbar m \left[e^{im\phi}\right]$

boundary conditions: $\Phi(0) = \Phi(2\pi)$ $\quad e^{im\cdot 2\pi} = 1$

$m = 0, \pm 1, \pm 2, \ldots$ $\qquad L_z = m\hbar$

deBroglie waves around Bohr orbitals!

- polar: $L^2\,\Theta(\theta) = \left[\frac{-\hbar^2}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{\hbar^2}{\sin^2\theta}\underbrace{\frac{\partial^2}{\partial\phi^2}}_{-m^2}\right]\Theta(\theta) = \hbar^2 l(l+1)\,\Theta(\theta)$

associated Legendre equation

* Group activity: test eigenvalues of eigenfunctions:

$m=0$: $\Theta(\theta) = 1$ $\qquad m=\pm 1$ $\Theta(\theta) = \cos(\theta)$, $\sin(\theta)$

$m=\pm 2$: $\Theta(\theta) = \frac{1}{2}(3\cos^2\theta - 1)$, $\sin\theta\cos(\theta)$, $\sin^2\theta$

* Summary: $Y_{lm}(\Omega) \propto P_{lm}(\cos\theta)\cdot e^{im\phi}$ "spherical harmonics"