L14-TISE: Separation of variables

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* Review: Time-Dependent Schrödinger equation (TDSE)
  - "operator-ized dispersion relation"

$$\hat{H}\Psi = \hat{E}\Psi \qquad \hat{H}(\hat{p},\hat{x}) = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x})$$

$$\left(\frac{\hat{p}^2}{2m} + \hat{V}\right)\Psi = \hat{E}\Psi \qquad \hat{p} = \hbar\hat{k} = -i\hbar\partial_x \qquad \hat{E} = \hbar\omega$$

- we constructed this from eigenfunction plane waves of the standard wave equation when $\hat{V}=0$:

$$\underbrace{\partial_x}_{\text{operator}} \underbrace{e^{ikx}}_{\text{eigenfunction}} = \underbrace{ik}_{\text{eigenvalue}} \underbrace{e^{ikx}}_{\langle x|k\rangle} \qquad \underbrace{\partial_t}_{\text{operator}} \underbrace{e^{-i\omega t}}_{\text{eigenfunction}} = \underbrace{-i\omega}_{\text{eigenvalue}} \underbrace{e^{i\omega t}}_{\langle t|\omega\rangle}$$

"tensor" product of eigenfunctions

$$\Psi(x,t) = e^{ikx} \cdot e^{i\omega t} \qquad \langle x,t|\,|k\rangle|\omega\rangle$$

- the general solution is a linear combination of (tensor) products of eigenfunctions: they form a basis of the solution space.

dispersion relation:

$$\Psi(x,t) = \int dk\, \Phi(k)\, e^{ikx-i\omega t} \sim \int \underbrace{dk}\, \Phi(k) \underbrace{|k\rangle}|\omega\rangle$$

only one "ω" per "k,.."

- coefficient $\Phi(k)$ from initial conditions

$$\langle k|\Psi_0\rangle = \langle k|\int dk'\,\Phi(k')\,|k'\rangle\cancel{|\omega'\rangle} = \int dk'\,\Phi(k')\cdot 2\pi\delta(k-k') = 2\pi\,\Phi(k)$$

$$\Phi(k) = \frac{1}{2\pi}\langle k|\Psi_0\rangle = \int dx\,\frac{1}{2\pi}e^{-ikx}\,\Psi(x,0) \qquad \hat{x}\cdot\vec{v} = v_x$$

* now apply the same technique to other potentials.
  - no longer plane waves, what about time-dependence?

- apply separation of variables to obtain new eigenfunctions.

$\Psi(x,t) = \psi(x)\cdot\varphi(t)$ $\quad \hat{H}|\psi\rangle = E|\psi\rangle \quad \hat{E}|\varphi\rangle = E|\varphi\rangle$

- if $\hat{H}$ is time-independent, $\hat{E}$ eigenfunctions already solved.

$\langle t|\hat{E}|\varphi\rangle = i\hbar\partial_t\varphi(t) = E\varphi(t)$ $\quad$ let $E = \hbar\omega$

$$\frac{d\varphi}{\varphi} = -i\omega\, dt \qquad \varphi(x) = \cancel{\varphi_0}\, e^{-i\omega t} = \cancel{\varphi_0}\, e^{-iEt/\hbar}$$

- the physics is in the $\hat{H}$ equation, the Time Independent Schrödinger Equation (TISE):

$$\hat{H}|\psi\rangle = E|\psi\rangle \qquad \left(\frac{-\hbar^2}{2m}\nabla^2 + \hat{V}\right)\psi_n(\vec{x}) = E_n\psi_n(x)$$

- Sturm-Liouville guarantees orthogonality: $\langle\psi_n|\psi_m\rangle = \underbrace{N_n^2}_{\text{normalization constant}}\delta_{nm}$

- general solution: $\Psi(x,t) = \sum_n \underbrace{c_n}_{\text{component}} \underbrace{\psi_n(x)\, e^{-iE_n t/\hbar}}_{\text{basis function}}$

- initial conditions: $\langle\psi_m|\Psi_0\rangle = \sum_n c_n\langle\psi_m|\psi_n\rangle = \cancel{N_m^2}\, c_m$ (normalized wavefunctions)

* formal solution to TDSE: (fancy representation of same steps!)

$$\hat{H}|\psi\rangle = \hat{E}|\psi\rangle = i\hbar\partial_t|\psi\rangle \qquad \hat{H}\,dt/i\hbar = d|\psi\rangle/|\psi\rangle$$

$$|\psi_t\rangle = \underbrace{e^{\hat{H}t/i\hbar}}_{\text{unitary } \hat{U}(t) \text{ time evolution operator}}|\psi_0\rangle = \overbrace{\sum_n e^{E_n t/i\hbar}|\psi_n\rangle}^{\text{spectral representation of } \hat{U}(t)}\underbrace{\langle\psi_n|\Psi_0\rangle}_{c_n}$$

* properties of $\psi_n(x)$: (Griffiths)

a) stationary states:

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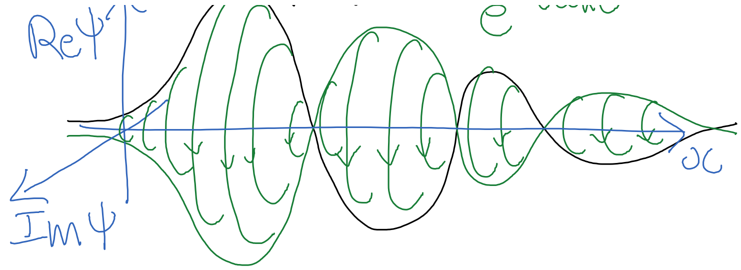
"skipping rope" function
like Bohr's orbitals



2-state system:

$$\Psi(x,t) = c_1 \psi_1(x) e^{iE_1 t/\hbar} + c_2 \psi_2(x) e^{-E_2 t/\hbar} \qquad \hbar \Delta\omega = E_2 - E_1$$

$$|\Psi(x,t)|^2 = |c_1|^2 \psi_1^2 + |c_2|^2 \psi_2^2 + 2|c_1^* c_2| \psi_1(x) \psi_2(x) \cos(\Delta\omega t)$$

exactly the Bohr frequency of transition radiation!

b) Energy eigenstates:
definite total energy

$$\langle \hat{H} \rangle = \langle \psi_n | \hat{H} | \psi_n \rangle = \langle \psi_n | E_n | \psi_n \rangle = E_n$$

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = 0 \qquad \langle f(\hat{H}) \rangle = f(E_n)$$

c) They form a complete set of states,
a basis of the Hilbert space

$$\sum_n |\psi_n\rangle\langle\psi_n| = I$$