L13-TISE: Separation of Variables

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

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

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

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x)\Psi = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

- we constructed this equation by converting the dispersion relation for free particles into an operator equation using the plane wave "eigenfunctions":

$$\underbrace{\partial_x}_{\text{operator}}\underbrace{e^{ikx}}_{\text{eigenfunction}} = \underbrace{ik}_{\text{eigenvalue}}\underbrace{e^{ikx}}_{|k\rangle} \qquad \underbrace{\partial_t}_{\text{operator}}\underbrace{e^{-i\omega t}}_{\text{eigenfunction}} = \underbrace{-i\omega}_{\text{eigenvalue}}\underbrace{e^{i\omega t}}_{|\omega\rangle} \qquad \Psi(x,t) = \underbrace{e^{ikx}\cdot e^{i\omega t}}_{\text{"tensor" product of eigenfunctions } |k\rangle|\omega\rangle}$$

- note the notation for operators "$\hat{p}$" and functions "$|k\rangle$", used to symbolize the linear nature (matrices & vectors).

- note: these functions are only solutions when $V(x)=0$.

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

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

dispersion relation: only one "ω" per "k,.."

- coefficient $\Phi(k)$ from initial conditions [don't worry about this yet!]

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

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

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

- apply separation of variables to obtain new eigenfunctions.

1) separate $\Psi(x,t) = \psi(x)\cdot\varphi(t)$ into product of functions.

2) separate x, t to separate sides of the PDE

$$\frac{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)\cancel{\varphi(t)} + V(x)\psi(x)\cancel{\varphi(t)}}{\psi(x)\cancel{\varphi(t)}} = \frac{i\hbar\frac{\partial}{\partial t}\cancel{\psi(x)}\varphi(t)}{\cancel{\psi(x)}\varphi(t)} = E$$

3) if $f(x) = g(t)$ then $f(x) = g(t) =$ constant, since each locks the other from changing
This is called the "constant of integration" or the "eigenvalue", depending on your point of view.
Write out each equation, multiplying out the denominator:

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\,\psi(x)}_{\text{Time Independent Schrödinger Eq. (TISE)}} \qquad \underbrace{i\hbar\frac{\partial}{\partial t}\varphi(t) = E\,\varphi(t)}_{\text{time equation.}}$$

- this only works for time-independent Hamiltonians $\hat{H}(x)$

- the constant E is the same in both equations.

* The time equation can be solved once for all times:

$$i\hbar\frac{d}{dt}\varphi(t) = E\,\varphi(t)$$

[this is an eigenvalue equation — we already know the solution!]

$$\int_0^{\varphi}\frac{d\varphi}{\varphi} = \int_0^t \frac{E}{i\hbar}\,dt$$

$$\ln\varphi = \frac{E}{i\hbar}\,dt \qquad \varphi(t) = \varphi_0\, e^{iEt/\hbar}$$

* A short-cut to separation of variables is to notice the eigenvalue equation early:

$$\hat{H}\,\Psi = \hat{E}\,\Psi = i\hbar\underbrace{\frac{\partial}{\partial t}}\,\Psi$$

[the only time dependence is $\frac{\partial}{\partial t}$]
the eigenfunction of $\frac{\partial}{\partial t}$ is $e^{i\omega t}$

$$\hat{H}\,\psi(x)\,e^{-i\omega t} = i\hbar(-i\omega)\,\psi(x)\,e^{-i\omega t}$$

$$\underbrace{\frac{\partial}{\partial t}}_{\text{operator}} e^{-i\omega t} = \underbrace{-i\omega}_{\text{eigenvalue}}\;\underbrace{e^{-i\omega t}}_{\text{eigenfunction}}$$

$$\hat{H}\,\psi(x) = \underbrace{\hbar\omega}_{\text{eigenvalue } E \text{ of } \hat{H}}\,\psi(x)$$

eigenvalue E of $\mathcal{H}$

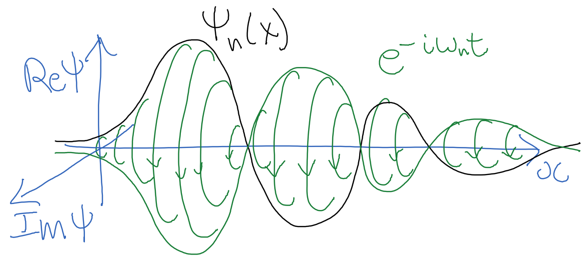
* Now we end up with a second eigenvalue equation $\hat{H}\psi = E\psi$, which we must solve for the eigenfunction $\psi(x)$.

  - The interesting physics is all in this T.I.S.E.:

$$\hat{\mathcal{H}}|\psi\rangle = E|\psi\rangle \quad \text{or} \quad \left(\frac{-\hbar^2}{2m}\nabla^2 + \hat{V}\right)\psi_n(\vec{x}) = E_n\psi_n(x) \quad (\text{in 3d})$$

* Just like eigenvectors, there are a whole series of independent "modes" or solutions to this equation, similar to the modes of E&M radiation in Rayleigh-Jeans theory.

properties of $\psi_n(x)$:



a) They are stationary states: "skipping rope" function
like Bohr's orbitals

All physical quantities are constant in time:

$$\langle Q(\hat{x},\hat{p})\rangle \equiv \langle \Psi_n | Q(x, -i\hbar\tfrac{\partial}{\partial x}) | \Psi_n\rangle \equiv \int dx\, \psi_n^*(x)\, \cancel{e^{i\omega_n t}}\, Q(x, -i\hbar\tfrac{\partial}{\partial x})\, \psi_n(x)\, \cancel{e^{-i\omega_n t}}$$

2-state system:

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar} \qquad \hbar\Delta\omega = E_2 - E_1$$

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

exactly the Bohr frequency of transition radiation!

b) They are energy eigenstates, having definite total energy:

$$\langle\hat{H}\rangle \equiv \langle\psi_n|\hat{H}|\psi_n\rangle \equiv \langle\psi_n|E_n|\psi_n\rangle = E_n \quad \text{likewise,} \quad \langle f(\hat{H})\rangle = f(E_n)$$

Thus the energy of these states is exact: $\sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2 = 0$

* Because the T.I.S.E. and both eigenequations are linear, we can form a general solution from the sum of individual solutions linked by E_n: (with arbitrary coefficients).

$$\Psi(x,t) = \sum_n \underbrace{c_n}_{\text{component}}\, \underbrace{\psi_n(x)\, e^{-iE_nt/\hbar}}_{\text{basis function}} \qquad \text{compare: } \vec{V} = \sum V_i\,\hat{e}_i = V_x\hat{x} + V_y\hat{y} + V_z\hat{z}$$

It looks a lot like a vector because it IS a vector! [linear]
Linear algebra theorems and techniques will help us solve every step along the way:

- Sturm-Liouville theory [eigensystems of continuous functions] guarantees a set of solutions of both eigenvalue equations:

a) they are "complete": $\boxed{\sum_n |\psi_n\rangle\langle\psi_n| = I}$
This guarantees that the general solution includes all others.

b) they are "orthogonal": $\boxed{\langle\psi_n|\psi_m\rangle = \delta_{nm}}$ (after normalization).
This provides a systematic method to determine the specific solution satisfying the initial conditions:

$$\int dx\, \psi_m(x)\, \Psi(x,0) \equiv \langle\psi_m|\Psi_0\rangle = \sum_n c_n \langle\psi_m|\psi_n\rangle = \sum_n c_n \delta_{nm} = c_m$$

Don't worry about the formalism yet – we will practice it in ch. 2 before the full formal treatment in Ch. 3.

Formal solution to TDSE: (fancy representation of same steps!) [skip!]

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

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