F. QM TISE is an Eigenvalue Problem: The Hamiltonian Operator

TDSE $$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x,t)\right]}\Psi(x,t) = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$$ general

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

For $U = U(x)$ only, $$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]}\psi(x) = E\psi(x)$$

$\boxed{\text{TISE}}$ $\boxed{\hat{H}\psi = E\psi}$

- Time-independent Schrödinger Equation is <u>an eigenvalue problem</u> of an operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$ [1D case]

Recall: Schrödinger (1926) solved his

$$\hat{H}\psi = E\psi$$

for H-atom, 1D oscillator, rotator

and found that E are the allowed energies of a system

and ψ_E are the states (wavefunctions) of definite energies E

$\therefore$ Expect $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$ to be related to the total energy of a system

What is that $\hat{H}$? A recipe to write down $\hat{H}$ for a quantum problem

- $\hat{H}$ is called the "Hamiltonian Operator" OR simply "Hamiltonian"
- Hamiltonian comes from classical mechanics = Hamilton's Mechanics

A minimal Picture of Classical Mechanics (physics is one big coherent subject)

- Classical Mechanics
  - Newton (1686) "Principia" $F = m\frac{d^2x}{dt^2}$
  - Lagrange (1787) "Analytic Mechanics"

Lagrangian → $L(x, \dot{x})$

$$\frac{d}{dt}\overbrace{\left(\frac{\partial L}{\partial \dot{x}}\right)}^{p} - \frac{\partial L}{\partial x} = 0$$ Euler-Lagrange Equation

gives equation of motion

  - Hamilton (1834) "On a general method on dynamics"

Hamiltonian → $H(x, p)$

$$\dot{p} = -\frac{\partial H}{\partial x} \; ; \; \dot{x} = \frac{\partial H}{\partial p}$$ Hamilton's Equations

give equation of motion

This page is meant to be formal – You ***don't*** need to go through these steps in most problems

But this will justify the sequence of learning: Classical Mechanics -> Quantum Mechanics

Given a problem (thus some $U(x)$ or some force) [we are doing classical mechanics]

1/. Identify coordinate x (called generalized coordinate)

2/. Construct Lagrangian $L(x, \dot{x})$

3/. Define momentum from L via $p = \frac{\partial L}{\partial \dot{x}}$ (conjugated momentum)

conjugate to coordinate x

4/. Construct $H(x,p) = p\dot{x} - L$

5/. Then we have $\underbrace{H(x,p)}$ formally, this is the Hamiltonian

it is a function of coordinate x and momentum p

(of coordinates x, y, z and momenta p_x, p_y, p_z)

Don't worry if your background doesn't fill in this page, **start with H directly is fine (next page)**

Practical Recipe: Writing $\hat{H}$

Step 1: Think Classical first

For most problems, H is the total energy and $H = H(x, p)$

i.e. $H = T + U$ = kinetic energy + Potential energy

$$\Rightarrow H = \underbrace{\frac{p^2}{2m}}_{\text{same for all 1D problems}} + \underbrace{U(x)}_{\text{specifies the problem}}$$

Example: A particle *m* confined by a harmonic potential (1D oscillator)

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}Kx^2$$

Up to this point, it is classical mechanics

Step 2: Go Quantum (this is the most important step)

- Turn coordinate x into an operator $\hat{x}$ (Position operator)
- Turn momentum p into an operator $\hat{p}$ (Momentum operator)
- Thus H becomes a Hamiltonian operator $\hat{H}$

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x})$$

- Recall x and p come in a pair (formally through $p = \frac{\partial L}{\partial \dot{x}}$)

  To get Schrödinger Equation:

  Substitute: $\hat{x} \to x$; $\hat{p} \to \frac{\hbar}{i}\frac{d}{dx}$ (crucial step into QM)

$^{+}$Recall: $\hat{p}\,\hat{p} \equiv \hat{p}^2$; $U(\hat{x})$ means for every x in $U(x)$, then it into $\hat{x}$

- Then $\hat{H}$ becomes

$$\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\text{kinetic energy term}} + \overbrace{U(x)}^{\text{potential energy function}}$$

- Time-independent Schrödinger Equation is given by (the eigenvalue problem)

$$\hat{H}\psi(x) = E\,\psi(x)$$

and thus $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\,\psi(x)$$

- Time-dependent Schrödinger Equation is

$$\hat{H}\,\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

Done! Steps 1 & 2 allow you to write down the QM equations for any system.
See Sample Questions and Problem Set 2 for practices.

- For 2D, 3D problems, follow the same recipe

Step 1 $H = T + U(x,y,z) = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + U(x,y,z)$

Step 2 coordinate $\leftrightarrow$ momentum pairs: $x \leftrightarrow p_x$; $y \leftrightarrow p_y$; $z \leftrightarrow p_z$

Go quantum: $\hat{x} \to x$ $\quad \hat{y} \to y$ $\quad \hat{z} \to z$

$\hat{p}_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}$ $\quad \hat{p}_y \to \frac{\hbar}{i}\frac{\partial}{\partial y}$ $\quad \hat{p}_z \to \frac{\hbar}{i}\frac{\partial}{\partial z}$

$$\hat{H} = \underbrace{\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)}_{\text{k.e. operator}} + U(x,y,z)$$

Done $\hat{H}\psi(x,y,z) = E\,\psi(x,y,z)$ TISE

Example: Harmonic Oscillator

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m}}_{\text{k.e.}} + \underbrace{\frac{1}{2}K\hat{x}^2}_{\text{potential energy function}}$$

TISE is $\hat{H}\psi(x) = E\psi(x)$ or $\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}Kx^2\psi(x) = E\psi(x)}$

Example: 3D harmonic Oscillator

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \frac{1}{2}K(\hat{x}^2 + \hat{y}^2 + \hat{z}^2)$$

$\hat{x} \to x$, $\hat{p}_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}$; $\hat{y} \to y$, $\hat{p}_y \to \frac{\hbar}{i}\frac{\partial}{\partial y}$; $\hat{z} \to z$, $\hat{p}_z \to \frac{\hbar}{i}\frac{\partial}{\partial z}$

TISE is $\hat{H}\psi = E\psi$ or $\boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) + \frac{1}{2}K(x^2+y^2+z^2)\psi(x,y,z) = E\psi(x,y,z)}$

One implication

$$H(x,p) = \underbrace{\frac{p^2}{2m}}_{T\text{ (kinetic energy)}} + U(x) \qquad [\text{Recipe} \Rightarrow \text{TISE}]$$

$$T = \frac{p^2}{2m} = \frac{1}{2}mv^2 \qquad \underbrace{\text{Newtonian}}_{\text{Meaning: Non-relativistic}}\text{, Mechanics}$$

$\therefore$ Schrödinger Equations : Non-relativistic Quantum Mechanics

Remarks: We will do non-relativistic QM in our course.
You may wonder how to do relativistic QM. That's "easy"! How about starting with $E^2 = m^2c^4 + c^2p^2$ and following the recipe? Klein, Gordon, and Dirac did just that and their equations are the starting points of relativistic QM

Making connections: Recall that...

Want to look for states of definite (some quantity) and values of (that quantity)?

Solve eigenvalue problem of (that quantity's) operator

Now that (some quantity) is the total energy of a system

Want to Look for states of definite energies and the values of energy?

Solve the eigenvalue problem of the $\underbrace{\text{total energy operator}}_{\text{Hamiltonian } \hat{H}}$

No wonder $\hat{H}\psi(x) = E\psi(x)$ gives the energy eigenfunctions (states of definite energies) and the energy eigenvalues (allowed energies of the system) This is what TISE does