II. The Wavefunction and the Wave Equation

- Background:
  - Need wave description for particle(s)
  - To proceed, introduced wavefunction $\Psi(x,t)$ or $\Psi(\vec{r},t)$
  - $|\Psi(x,t)|^2 dx$ = Prob. of finding particle in interval x to $x+dx$ at time t

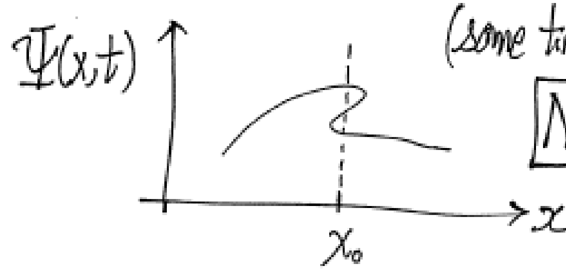
Questions†:

- What do we expect $\Psi(x,t)$ to behave based on physics?
- If we somehow know $\Psi(x,t)$, how to use it for calculations?
- What is the governing wave equation for $\Psi(x,t)$?

† We use $\Psi(x,t)$ here for easy visualization. Discussions also are valid for $\Psi(\vec{r},t)$.

A. Some expected behavior of $\Psi(x,t)$ based on physics

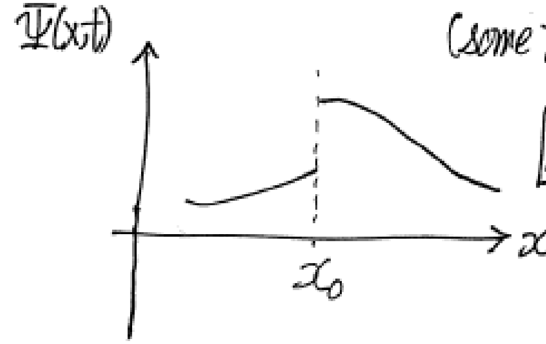
- Single-value:



(some time t)

$\boxed{\text{NO}}$ (illegal)

- Continuous:



(some time t)

$\boxed{\text{NO}}$ (illegal)

Can't tell probability[+] of finding particle at x_0

- Can Ψ be negative? YES!
- Can Ψ be complex? YES!

Physical Meaning is attached to $|\Psi(x,t)|^2$

[+] Here, we use physical sense. Continuity requirement can also be shown mathematically, after knowing the wave equation. Single-valueness applies almost in all cases (except strange spin situations).

B. Normalization

- Formal statement

  - $|\Psi(x,t)|^2 dx$ = Prob. of finding particle in $x \to x+dx$ at time t
  - Particle is there and cannot be destroyed (or more being created)

    Eg. H-atom

"know" electron to be around

$\Psi(\vec{r},t)$ describes state of electron

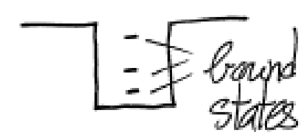
  - $\displaystyle\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$ or $\displaystyle\int_{\text{all space}} |\Psi(\vec{r},t)|^2 d^3r = 1$ [Eq.(1)]

Practically, it means that $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx$ = finite, then $\Psi(x,t)$ can be <u>normalized</u>

Practical Tips

- In a large class of QM problems on studying <u>bound states</u> [states with $\psi \to 0$ as $x \to \pm\infty$ (fast enough)], the <u>wavefunctions of bound states can be normalized</u>.

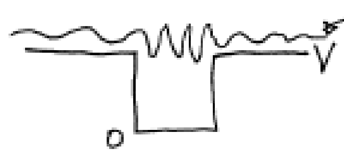
  <u>E.g.</u>: all states in an infinite well & harmonic oscillator

  states with energies lower than $V(\pm\infty)$ as in 

  and in atomic states with energy < 0

  $\therefore$ We will make use of normalization requirement in bound states in
  - 1D infinite and finite wells, 1D harmonic oscillator
  - 2D wells, rotor
  - 3D wells, Hydrogen atom, other atoms, molecules

- But there are solutions of Schrödinger Equation that are <u>NOT</u> bound states!

E.g. 

a state with $E > V$ (called scattering state)

- These states cannot be normalized as in Eq.(1)
- But these states are sometimes useful

<u>What to do then?</u> There are several ways out!

- Use $\underbrace{\text{wave packet}}_{\text{formed by adding up unbounded states (c.f. Fourier)}}$  to describe particle

  localized in a range of space

- "Normalized" them differently (not as Eq.(1))
- Let space be <u>big</u> <u>but</u> <u>finite</u> (often use in Solid State Physics)

- Key Points
  - In handling bound states in QM, need to consider normalization
  - Don't worry too much about unbound states, until it is absolutely necessary.
- Appreciation
  - In classical physics, $\vec{E}(x,t)$ and $10\cdot\vec{E}(x,t)$ are different, different intensities
  - In QM bound states, $\Psi(x,t)$ and $10\cdot\Psi(x,t)$ are the "same".
    They give the same information on prob. at x to $x+dx$. Only one is normalized and another is not properly normalized (but can be normalized)

$$\int_{-\infty}^{\infty} \left|\Psi^{\text{not normalized}}(x,t)\right|^2 dx = A \quad (\underline{\text{finite}}) \qquad [\text{still fine, no problem}]$$

Construct: $\Psi(x,t) = \dfrac{1}{\sqrt{A}}\, \Psi^{\text{not normalized}}(x,t)$

[This step is called normalization]

this is now properly normalized as

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \frac{1}{A}\int_{-\infty}^{\infty} \left|\Psi^{\text{not normalized}}(x,t)\right|^2 dx = \frac{1}{A}\cdot A = 1$$

As long as A is ***finite*** (not infinite), the wavefunction can be normalized.

Summary: For a normalized wavefunction

$|\Psi(x,t)|^2 dx$ = Prob. of finding particle in $x \to x+dx$ at time t

and a similar interpretation in 2D and 3D

- Probabilistic interpretation:

Max Born [Nobel Prize 1954]

Heisenberg was Born's RA after graduation. During which Heisenberg, Born, Kramer, Jordan wrote the first papers on QM in 1924-25. Heisenberg was awarded the 1932 Nobel Prize (Born was left out).

Max Born (1882-1970)

Other contributions include:

- Mentored Heisenberg even before he graduated from Munich with a thesis on turbulence (with Sommerfeld)
- Took Heisenberg's idea to Hilbert (Born and Hilbert were both at Gottingen), helped establish the mathematical foundation of QM
- Born-Oppenheimer approximation (molecular physics)
- Born-Huber cycle (thermodynamics, chemistry)
- Born approximation (QM scattering theory)
- Born and (Kun) Huang (lattice vibrations in solid state physics) [Kun Huang trained generations of semiconductor physicists in China]