Summary

Time Evolution: (time independent Hamiltonian)

Method 1:
Solution via Energy Eigenstates:

Step 1: find eigenvectors $|E_n\rangle$ and eigenvalue E_n of H

Step 2: Expand initial state in eigenbasis

$$|\Psi(0)\rangle = \sum_n c_n \, |E_n\rangle$$

Step 3: Write down solution

$$|\Psi(t)\rangle = \sum_n c_n \, e^{-i\frac{E_n t}{\hbar}} \, |E_n\rangle$$

Method 2:
Calculate unitary time evolution operator

Step 1: find eigenvectors $|E_n\rangle$ and eigenvalue E_n of H

Step 2: calculate time evolution operator:

$$U(t) = \sum_n e^{-\frac{i}{\hbar}E_n t} \, |E_n\rangle\langle E_n|$$

$$U(t) = e^{-\frac{i}{\hbar}Ht}$$

Step 3: Write down solution

$$|\Psi(t)\rangle = U(t) \, |\Psi(0)\rangle$$

	Discrete	Continuous
State	$\vert\Psi\rangle$	$\vert\Psi\rangle$
coordinate representation	$\vert\Psi\rangle \doteq \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{pmatrix}$	$\vert\Psi\rangle \doteq \langle x\vert\Psi\rangle =: \Psi(x)$ wavefunction (complex valued!) (position representation)
completeness relations	$\mathbb{1} = \sum_{k=1}^{n} \vert\phi_k\rangle\langle\phi_k\vert$ orthonormal basis	$\mathbb{1} = \int_{-\infty}^{+\infty} dx\ \vert x\rangle\langle x\vert$ position states
dual vector	$\langle\Psi\vert \doteq (\ \Psi_1^*,\ \ldots\ \Psi_n^*\ )$	$\langle\Psi\vert \doteq \langle\Psi\vert x\rangle = \Psi(x)^*$
scalar product	$\langle\Phi\vert\Psi\rangle = \sum_{k=1}^{n} \Phi_k^*\Psi_k$	$\langle\Phi\vert\Psi\rangle = \int_{-\infty}^{+\infty} dx\ \Phi(x)^*\Psi(x)$
normalization	$1 \stackrel{!}{=} \langle\Psi\vert\Psi\rangle = \sum_{k=1}^{n} \vert\Psi_k\vert^2$	$1 \stackrel{!}{=} \langle\Psi\vert\Psi\rangle = \int_{-\infty}^{+\infty} dx\ \vert\Psi(x)\vert^2$
probability prediction	$\Pr(\text{"k"}) = \vert\langle\phi_k\vert\Psi\rangle\vert^2 = \vert\Psi_k\vert^2$ probability	$p(x)\ dx = \vert\langle x\vert\Psi\rangle\vert^2\ dx = \vert\Psi(x)\vert^2\ dx$ probability density

Position Operator

$\hat{X} = \int_{-\infty}^{+\infty} dx\ x\vert x\rangle\langle x\vert$

eigenvector: $\hat{X}\vert x\rangle = x\vert x\rangle$

(position) coordinate representation:

$$\hat{X} \doteq x\ \delta(x-x')$$
$$\vert x\rangle \doteq \Psi(x') = \langle x'\vert x\rangle = \delta(x-x')$$
$$\hat{X}\vert\Psi\rangle \doteq x\Psi(x)$$

Momentum Operator

$\hat{P} = \int_{-\infty}^{+\infty} dp\ \ p\vert p\rangle\langle p\vert$

eigenvector: $\hat{P}\vert p\rangle = p\vert p\rangle$

(position) coordinate representation:

$$\hat{P} \doteq (-i)\hbar\ \tfrac{d}{dx}\ \delta(x-x')$$
$$\vert p\rangle \doteq \Psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\exp[\frac{ipx}{\hbar}]$$
$$\hat{P}\vert\Psi\rangle \doteq (-i)\hbar\frac{d}{dx}\Psi(x)$$

General Coordinate Representation Rule

$$\begin{aligned} \vert\Psi\rangle &= \int_{-\infty}^{+\infty} dx\ \Psi(x)\vert x\rangle &&\doteq \Psi(x) \\ \hat{A} &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dx\ dx'\ g(x,x')\vert x\rangle\langle x'\vert &&\doteq g(x,x') \\ \langle\Phi\vert &= \int_{-\infty}^{+\infty} dx\ \Phi^*(x)\langle x\vert &&\doteq \Phi^* \end{aligned}$$

$$\begin{aligned} \Psi(x) &= \langle x\vert\Psi\rangle \\ g(x,x') &= \langle x\vert\hat{A}\vert x'\rangle \\ \Phi^*(x) &= \langle\Phi\vert x\rangle \end{aligned}$$

$$\begin{aligned} \langle\Phi\vert\Psi\rangle &= \int_{-\infty}^{+\infty} dx\ \ \Phi^*(x)\Psi(x) \\ \hat{A}\vert\Psi\rangle &\doteq \int_{-\infty}^{+\infty} dx' g(x,x')\Psi(x') \\ \langle\Phi\vert\hat{A}\vert\Psi\rangle &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dx\ dx'\ \Phi^*(x)g(x,x')\Psi(x') \end{aligned}$$

Solving Strategies: time evolution of free particle

$$\boxed{\frac{d}{d\,t}|\Psi(t)\rangle = -\frac{i}{\hbar}H|\Psi(t)\rangle}$$

Initial state: $|\Psi(0)\rangle$ mass: m

1) Find Eigensystem of H:

$\hat{H} = \frac{\hat{P}^2}{2m}$ eigenstates: $|p\rangle$, p in ($-\infty$, $+\infty$) eigenvalues: $E = \frac{p^2}{2m}$ degenerate

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_E(x) = E\Psi(x)_E$$

solution: $|p\rangle \doteq \frac{1}{\sqrt{2\pi\hbar}}\exp(i\frac{px}{\hbar})$

2) Decompose initial state into eigenstates of H

$$|\Psi(0)\rangle = \int dp\ \langle p|\Psi(0)\rangle\ |p\rangle$$

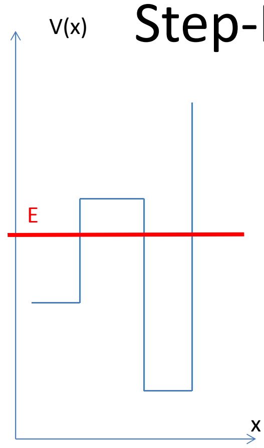
$$\begin{aligned}\Psi_p(p,0) &= \langle p|\Psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int dx\ \Psi(x,0)\exp(-i\frac{xp}{\hbar})\end{aligned}$$

3) Write down final solution

$$|\Psi(t)\rangle = \int dp\ \langle p|\Psi(0)\rangle\ e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}|p\rangle$$

$$\boxed{\Psi(x,t) = \int dp\ \Psi_p(p,0)\ e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}\frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{xp}{\hbar}}}$$

Step-Potentials: Eigenstates



1) Mathematical Ansatz in each section

$$\Psi_E(x) = \begin{cases} A_+\ e^{\kappa x} + A_- e^{-\kappa x} & E < V_0 \\ B_+\ e^{ikx} + B_-\ e^{-ikx} & E > V_0 \end{cases}$$

$$\kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)} \qquad k = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$$

2) Physical constraint

no exponential growth as $|x| \to \infty$

3) Matching conditions at interfaces

finite jumps: $\Psi_E(x)$ and $\frac{d}{dx}\Psi_E(x)$ continuous

infinite jumps: $\Psi_E(x)$ continuous, while $\frac{d}{dx}\Psi_E(x)$ may make finite jump

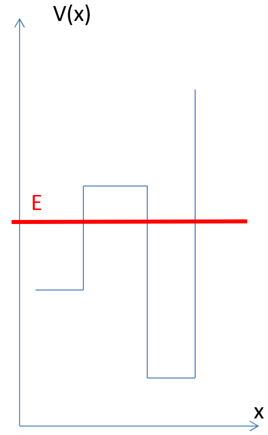
4) Normalization

discrete spectrum $\langle E_n|E_n\rangle = 1$

continuous spectrum $\langle E_n|E_m\rangle = \delta(E_n - E_m)$

Optional:
symmetric potential with respect to some x_0:
➔ each energy eigenstate is either symmetric or anti-symmetric with respect to x_0

Result classes for N sections



Step 1: Mathematical Ansatz
each section has 2 complex amplitude parameters
➔ 2N parameters
Step 2: Physical constraints (0,1,or 2 constraints)
for each section with $|x| \to \infty$
one complex amplitude is set to 0!
➔ number of affected sections C_{ph}
Step 3: interfaces ➔ 2(N-1) constraints
finite jumps:
2 linear homogeneous constraints on amplitudes
(wave function and derivative continuous)
infinite wall:
2 linear homogeneous constraints on amplitudes
(wave function continuous,
amplitude in infinite potential zero)

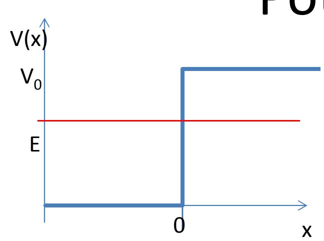
➔ 2N parameters
➔ C_{tot} = 2(N-1) + C_{ph} constraints!

C_{tot} = 2N
➔ bound states
➔ discrete spectrum
➔ non-degenerate

C_{tot} = 2N-1
➔ unbound state
➔ continuous spectrum
➔ non-degenerate

C_{tot} = 2N-2
➔ unbound state
➔ continuous spectrum
➔ degenerate

Potential Step



<u>Eigenstates of Hamiltonian</u>

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + V(\hat{X})$$

<u>Eigenstates for energy eigenvalue range $0<E<V_0$</u>
non-degenerate continuous eigenvalues:

$$\Psi_E(x) = A_+ \begin{cases} e^{ikx} + \frac{k-i\kappa}{k+i\kappa} e^{-ikx} & x \leq 0 \\ \frac{2k}{k+i\kappa} e^{-\kappa x} & x > 0 \end{cases}$$

$$\kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$$

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

<u>Eigenstates for energy eigenvalue range $E>V_0$</u>
Degenerate continuous eigenvalues:

<u>Flux ONLY from $-\infty$:</u>

$$\Psi_E(x) = A_+ \begin{cases} e^{ik_1 x} + \frac{k_1-k_2}{k_1+k_2} e^{-ik_1 x} & x \leq 0 \\ \frac{2k_1}{k_1+k_2} e^{ik_2 x} & x > 0 \end{cases}$$

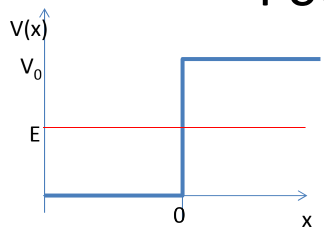
<u>Flux ONLY from $+\infty$:</u>

$$\Psi_E(x) = \begin{cases} \ldots & x \leq 0 \\ \ldots & x > 0 \end{cases}$$

$$k_1 = \frac{1}{\hbar}\sqrt{2mE}$$

$$k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$$

Potential Step



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Degenerate continuous eigenvalues:

Flux ONLY from - ∞:

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Flux ONLY from + ∞:

$$\Psi_E(x) = \begin{cases} \ldots & x \leq 0 \\ \ldots & x > 0 \end{cases}$$

$$k_1 = \frac{1}{\hbar}\sqrt{2mE}$$

$$k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$$

Probability Flux

$A_+ e^{i(kx - \frac{Et}{\hbar})}$

$A_- e^{i(-kx - \frac{Et}{\hbar})}$

$k = \frac{1}{\hbar}\sqrt{2m(E-V)}$

$B_+ e^{i(k'x - \frac{Et}{\hbar})}$

$k' = \frac{1}{\hbar}\sqrt{2m(E-V')}$

Probability flux for each component:
(applies only for E > V(x)!)

$$S_{comp} = \frac{\hbar}{m} k |A|^2$$

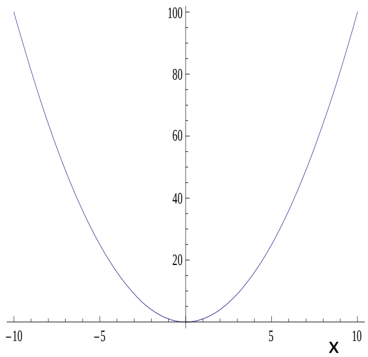
Reflection probability:

$$R = \frac{S_{reflect}}{S_{in}} = \frac{|A_-|^2}{|A_+|^2}$$

Transmission probability:

$$T = \frac{S_{transmit}}{S_{in}} = \frac{k'}{k}\frac{|B_+|^2}{|A_+|^2}$$

Harmonic Oscillator



$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{X}^2$$

$$[\hat{X},\hat{P}] = i\hbar\,\mathbb{1}$$

$$\hat{H} = \hbar\omega\,\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\mathbb{1}\right)$$

$$\hat{N} = \hat{a}^\dagger\hat{a} \qquad \hat{N}|n\rangle = n\,|n\rangle$$

$$\hat{H}|n\rangle = \hbar\omega(n+1/2)\,|n\rangle$$

n=0,1,2,3 ...

ladder operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{X} + \frac{i}{m\omega}\hat{P}\right)$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{X} - \frac{i}{m\omega}\hat{P}\right)$$

commutator:

$$\left[\hat{a},\hat{a}^\dagger\right] = \mathbb{1}$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$$

PHYS 234: Quantum Physics I

Norbert Lütkenhaus
Institute for Quantum Computing & Dept. Physics and Astronomy

Richard Feynman:
"I think I can safely say that nobody understands quantum mechanics."

John Wheeler:
"If you are not completely confused by quantum mechanics, you do not understand it."

But what does it mean to "understand"?

"Understanding"

Formulation of rules

➔ correct prediction of outcomes of experiments
➔ prediction of new effects

What are the underlying principles of these rules? (minimal assumptions)
➔ simplification of rules
➔ formulate new theories

Why are the rules the way they are?

Classical Mechanics:

Newton's law + …

Variational Principle
(Lagrange & Hamiltonian Formulation)
➔ Field Theory

Interesting philosophical question

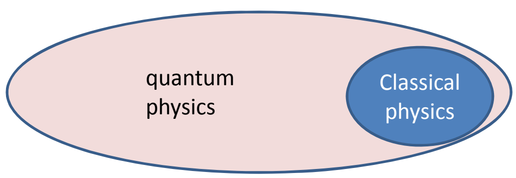
Quantum Mechanics (QM):

Formalism of QM clear ➔ works great!

Research in Progress
➔ attempt to formulate principles without reference to math structure

Interesting philosophical question …

Quantum Mechanics vs. Classical Physics



Many notions of classical physics will become obsolete in quantum physics
➔ they emerge only in some limit (classical limit)

classical physics:
objects have always well defined position and momentum

quantum physics:
no simultaneous position and momentum measurement
➔ cannot put one particle into one spot

a measurement does not simply reveal a pre-existing value …

Nils Bohr:
"For those who are not shocked when they first come across quantum theory cannot possibly have understood it."