1D quantum summary

Wave-particle duality
massless particle (photon) $E = \hbar \omega$ $p = 2\pi\hbar / \lambda$
Massive particles — deBroigle wavelength
$$\lambda = \frac{2\pi\hbar}{P}$$ (non-relativistic) $p = mv$
$$K = \frac{mv^2}{2} = p^2/2m$$

Wave function: describes the quantum state of a particle, obeys general Schrodinger equation
$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t)$$

A wave function is not measurable, it is an intellectual construction. Physically measurable value is probability density $P(x,t) = |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$
(here * means complex conjugation)
Probability density $P(x,t)$ describes the probability of detecting a quantum object at point x at time t.
Probability of detection of particle $a < x < b$
$$\int_a^b P(x,t)\, dx = \int_a^b |\Psi(x,t)|^2\, dx$$
For bound states (localized particles) $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx = 1$
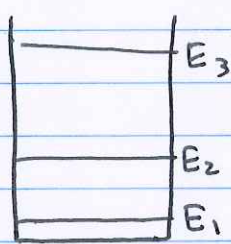(normalization)

Quantum superposition: a particle can be in superposition of several defined quantum states
$$\Psi(x,t) = C_1 \Psi_1(x,t) + C_2 \Psi_2(x,t) + \ldots$$

The probability to find a particle in one of these states $\Psi_i(x,t)$ is defined by the coefficient $P_i = |C_i|^2$

Examples of potential

a) Infinite square well

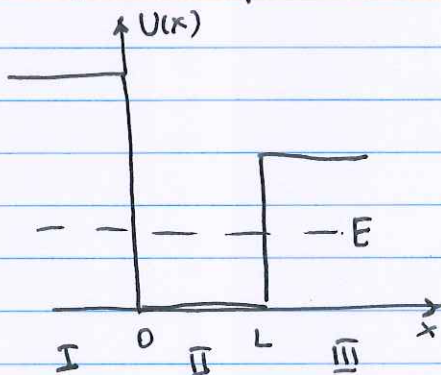$$U(x) = \begin{cases} \infty & x<0, x>L \\ 0 & 0<x<L \end{cases}$$

$E_3$, $E_2$, $E_1$

$$E_n = \frac{\pi^2 t^2 \hbar^2}{2mL^2}$$

$$\psi_n = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} & 0<x<L \\ 0 & x<0 \quad x>L \end{cases}$$

This energy spectrum can be derived from the boundary conditions $\psi(0) = \psi(L) = 0$

b) Finite potential well

$U(x)$

$$U(x) = \begin{cases} U_1 & x<0 \\ 0 & 0<x<L \\ U_2 & x>L \end{cases} \qquad \begin{array}{l} E < U_1, U_2 \\ \text{bound state} \end{array}$$

$-.E$

$$\psi(x) = \begin{cases} Ce^{d_1 x} & x<0 \\ A\cos kx + B\sin kx & 0<x<L \\ De^{-d_2 x} & x>L \end{cases}$$

I   0   II   L   III   $x$

I, III — classically forbidden
regions    $E < U(x)$
II  — classically allowed
region    $E > U(x)$

From Schrodinger equation
$$k = \sqrt{2mE/\hbar^2}, \quad d_1 = \sqrt{2m(U_1-E)/\hbar^2}$$
$$d_2 = \sqrt{2m(U_2-E)\hbar^2}$$

$\psi(x)$ must be smooth and
continuous at $x=0$, $x=L$ =>

These boundary conditions will provide a system
of linear equations for coefficients A, B, C, D and
energy E, which can be used to derive
a transendental equation containing only
k-s and d-s, that, if solved numerically,
will define descrete energy values, corresponding
to stationary states.

c) Harmonic potential $U(x) = \frac{1}{2} m\omega^2 x^2$

Characteristic equidistant spectrum ~~$E_n = \frac{1}{2} \hbar \omega$~~
$$E_n = \hbar\omega \left(n + \frac{1}{2}\right)$$
ground state (i.e. the state with the lowest energy ) is $n=0$ $\quad E_0 = \frac{1}{2}\hbar\omega$

<u>Unbound states</u> : no restrictions on particle energy for a stationary state (continuous spectrum)
In these problems we usually look for transmission and reflection coefficients

incoming →

→ transmitted

← reflected

quantum black box
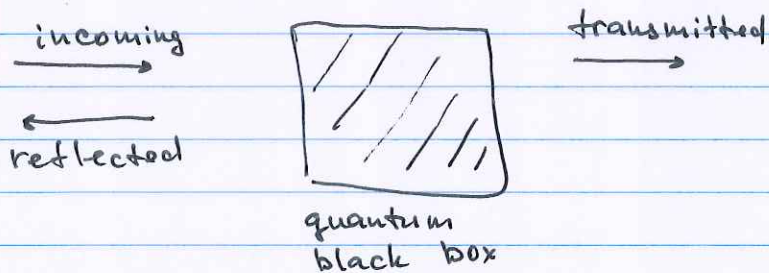
Away from the box we can use complex exponents to understand which wave is ~~voted~~ which:
$e^{ikx}$ — a particle flux along x-axis
$e^{-ikx}$ — a particle flux ~~away~~ against x-axis

Typically one one side: $\psi(x) = A e^{ikx} + B e^{-ikx}$
$\qquad\qquad\qquad\qquad\qquad$ incoming $\quad$ reflected

and on the other side $\quad \psi(x) = C e^{ikx}$
$\qquad\qquad\qquad\qquad\qquad\qquad$ transmitted

Reflection coefficient (probability) $\quad R = \left|\frac{B}{A}\right|^2$
Transmission coefficient $\quad T = 1-R \quad$ or $\quad T = \left|\frac{C}{A}\right|$
(if the potential energy is the same on both sides)

Each step in the potential produces reflection:
in the classically-allowed region it is a real running wave ($e^{\pm ikx}$); in a classically forbidden region it is the evanescent wave ($e^{\pm dx}$)

We are mostly focussed of finding stationary states for each potential energy profile ( we usually just call it "potential" )

These states correspond to well-defined value of particle's total energy $E$, and the corresponding wave functions are the solutions of time-independent Schrodinger equation:

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

Time-evolution of these states is known:

$$\psi(x,t) = \underset{\text{Stationary}}{\psi(x)}\, e^{-iEt/\hbar}$$

If the motion of a classical particle is restricted to a certain region ( quantum well ), only some values of total energy $E_n$ will allow stationary states $\psi_n(x)$.

For each state $\psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$

If at $t=0$ a particle is in the super position of several stationary states

$$\psi(x) = C_1\psi_1(x) + C_2\psi_2(x) + \dots$$

Then we can figure out its time evolution without solving the general Schrodinger equation

$$\psi(x,t) = C_1\psi_1 e^{-iE_1 t/\hbar} + C_2\psi_2 e^{-iE_2 t/\hbar} + \dots$$

and the probability of finding the particle in one of those states- n (with energy $E_n$) is $\quad P_n = |C_n|^2$