PHYS-C0252 - Quantum Mechanics Part 2
Sections 4.1-4.2

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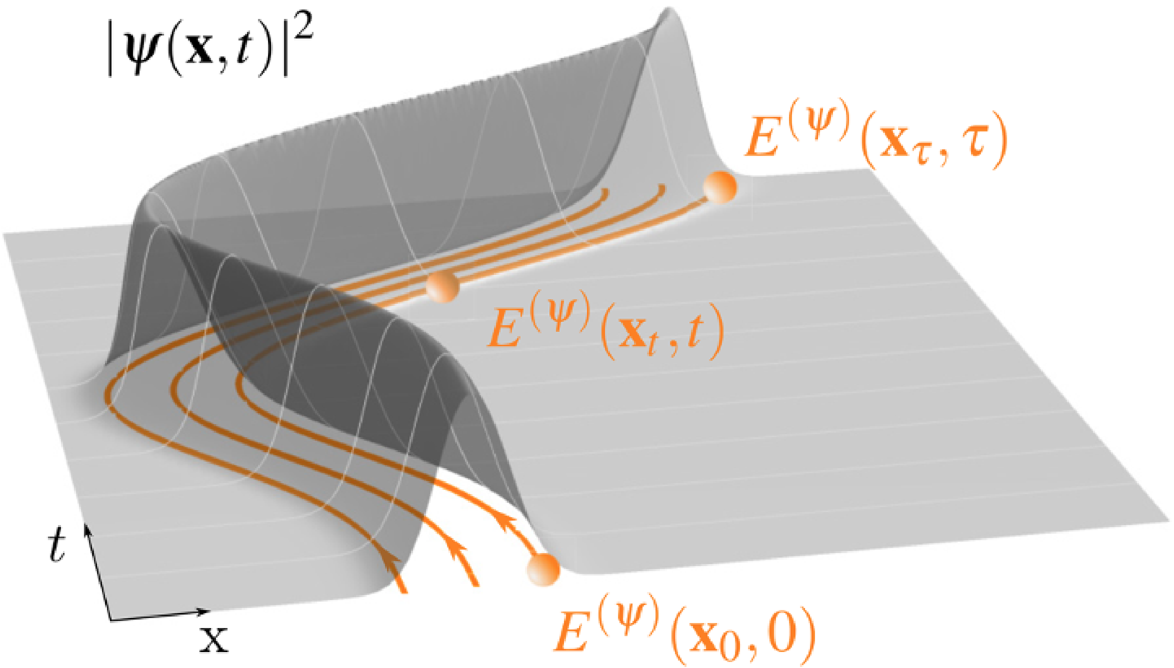
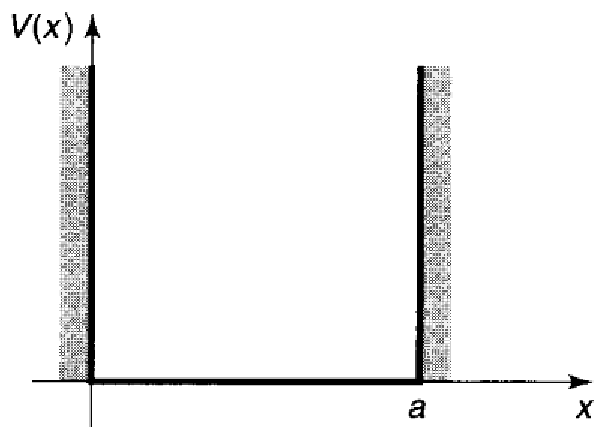


4. Particles in External Potentials
4.1 Infinite Potential Well

- The simplest case is that of a particle confined between two infinite walls, where



$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a, \\ \infty, & \text{otherwise} \end{cases}$$

Since there's no potential in the well, the solution of the SE is that of a free particle

$$\psi''(x) = -k^2\psi(x), \ k = \frac{\sqrt{2mE}}{\hbar}$$

This is the classical HO, whose solutions are

$$\psi(x) = A \sin kx + B \cos kx$$

Continuity requires that $\psi(0) = \psi(a)$ and thus *B* = 0, and because the function must be zero at boundaries

$$\psi(x) = A \sin kx, \;\; ka = 0, \pm\pi, \pm 2\pi, ...$$

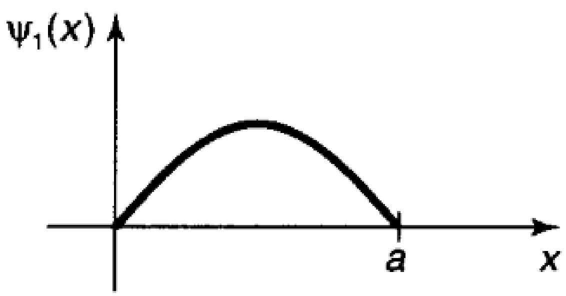
i.e. $k_n = n\pi/a \; (n \in \mathbb{Z})$ which means that the energy is quantized as

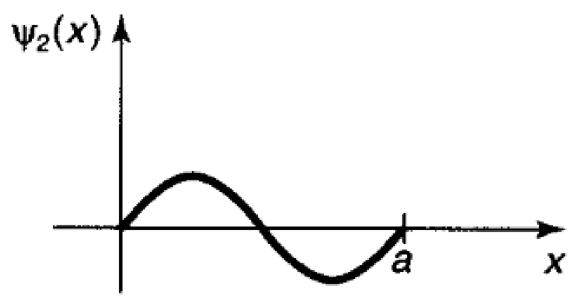
$$E_n = \frac{\hbar^2 k_n^2}{2m}$$

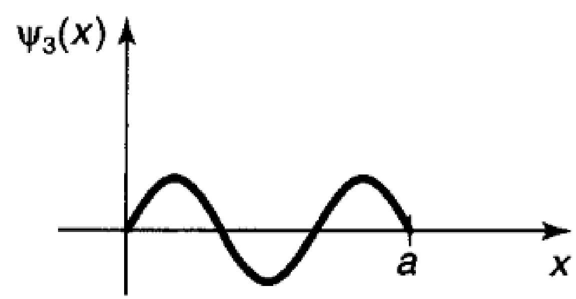
Normalization of the wave function gives easily

$$A = \sqrt{2/a}$$

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right),\ n \in \mathbb{Z}$$







The stationary states of the time-dependent SE are given by (cf. Section 2):

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-\imath E_n t/\hbar}$$

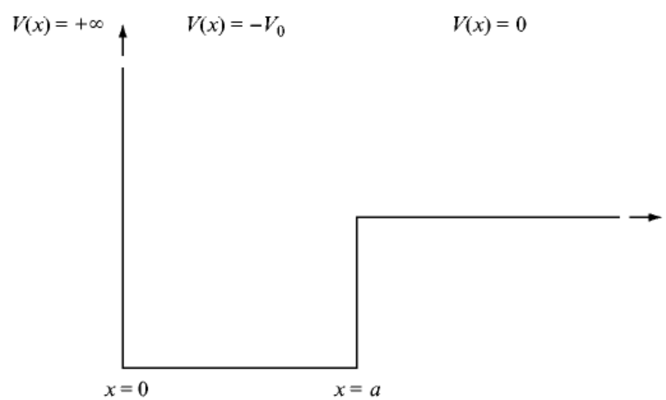
Then the most general solution to the time-dependent SE can be written as

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-\imath E_n t/\hbar}$$

where the expansion coefficients depend on the initial state $\Psi(x,0)$

4.2 Square-Well Potential

- Another simple example is that of a particle in a square-well potential:



$$V(x) = \begin{cases} \infty & \text{if } -\infty < x < 0 \\ -V_0 & \text{if } 0 < x < a \\ 0 & \text{if } a < x < \infty. \end{cases}$$

There are now two types of solutions: *bound* states whose energy is below zero and *unbound* (free) states. For $x < 0$, $\psi(x) = 0$

For bound states $0 < x < a$

$$\psi''(x) = -k_0^2\psi(x), \;\; E = \frac{\hbar^2 k_0^2}{2m} - V_0$$

whose (continuous) solution is $\psi(x) = C\sin k_0 x$

- In the final region *x* > *a,* the free particle solution applies (but with negative energy):

$$\psi''(x) = k^2\psi(x), \;\; k^2 = -\frac{2mE}{\hbar^2}$$

Now the general solution is $\psi(x) = Ae^{-kx} + Be^{kx}$ where *B* = 0 (why?)

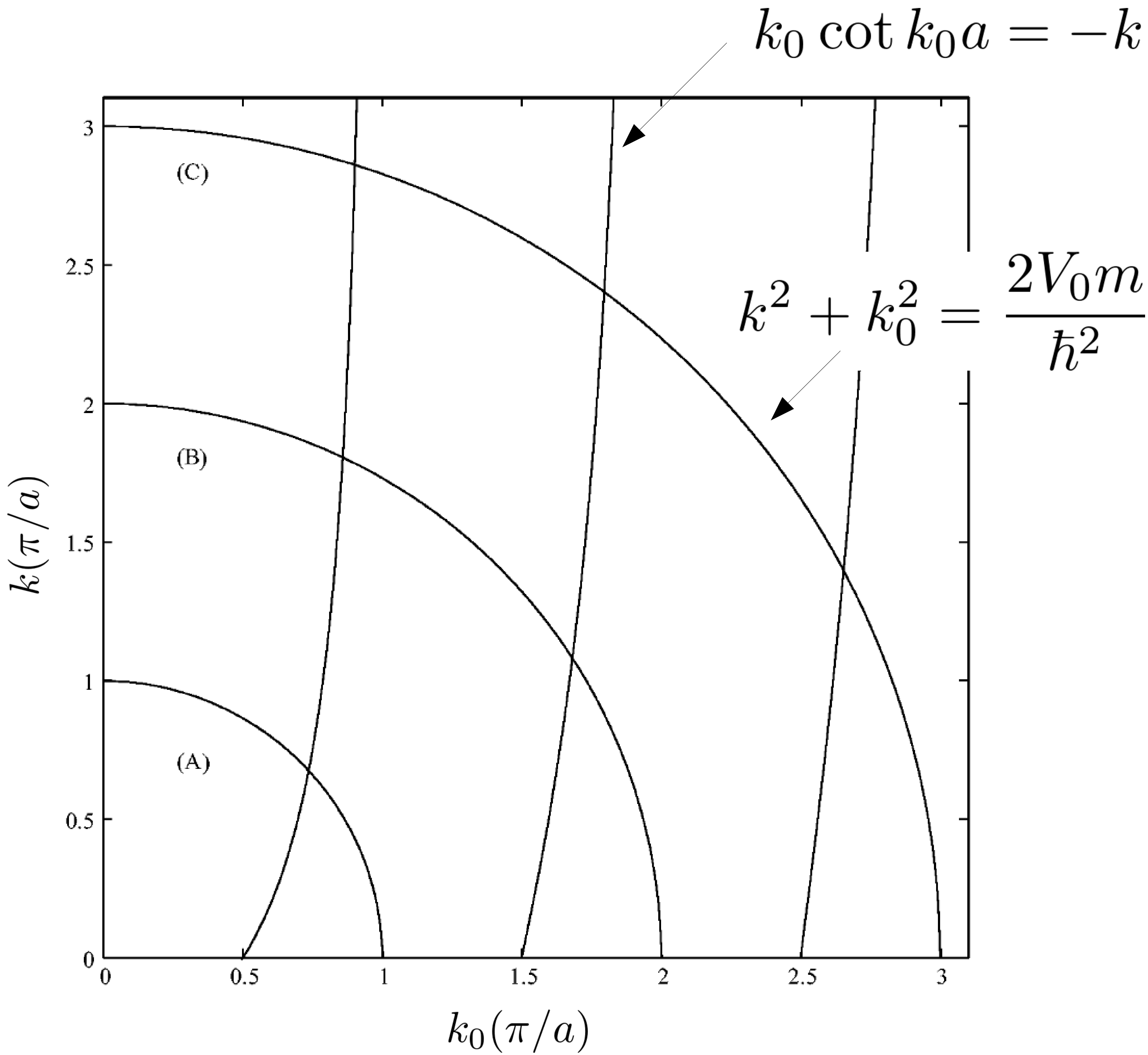
- The continuity of $\psi(a)$ and $\psi'(a)$ requires that

$$k_0 \cot k_0 a = -k^2$$

Because both variables depend on the energy, they have to satisfy

$$k^2 + k_0^2 = \frac{2V_0 m}{\hbar^2}$$

For solutions (bound states) to exist, these two equations have to match:


$k_0 \cot k_0 a = -k$
$k^2 + k_0^2 = \frac{2V_0 m}{\hbar^2}$
(C)
(B)
(A)
$k(\pi/a)$
$k_0(\pi/a)$
0
0.5
1
1.5
2
2.5
3

For the *unbound* states the wave function is again zero for $x < 0$. For $0 < x < a$, the bound state equation turns into

$$\psi''(x) = -k_0^2 \psi(x), \;\; E = \frac{\hbar^2 k_0^2}{2m} - V_0$$

with solution $\psi(x) = C \sin k_0 x$

In the last region $a < x < \infty$

$$\psi''(x) = -k^2 \psi(x), \;\; E = \frac{\hbar^2 k^2}{2m}$$

and we need to include phase shift

$$\psi(x) = D \sin(kx + \delta)$$

The continuity condition at *a* now gives

$$k_0 \cot k_0 a = k \cot(ka + \delta)$$

Unlike for the bound states, there's a smooth eigenfunction for any energy value as

$$\psi(x) = \begin{cases} 0 & \text{if } -\infty < x < 0 \\ C \sin(k_0 x) & \text{if } 0 < x < a \\ D \sin(kx + \delta) & \text{if } a < x < \infty. \end{cases}$$

By defining

$$A_0 = -\frac{C}{2i} \quad \text{and} \quad A = -\frac{D\,\mathrm{e}^{-2i\delta}}{2i}$$

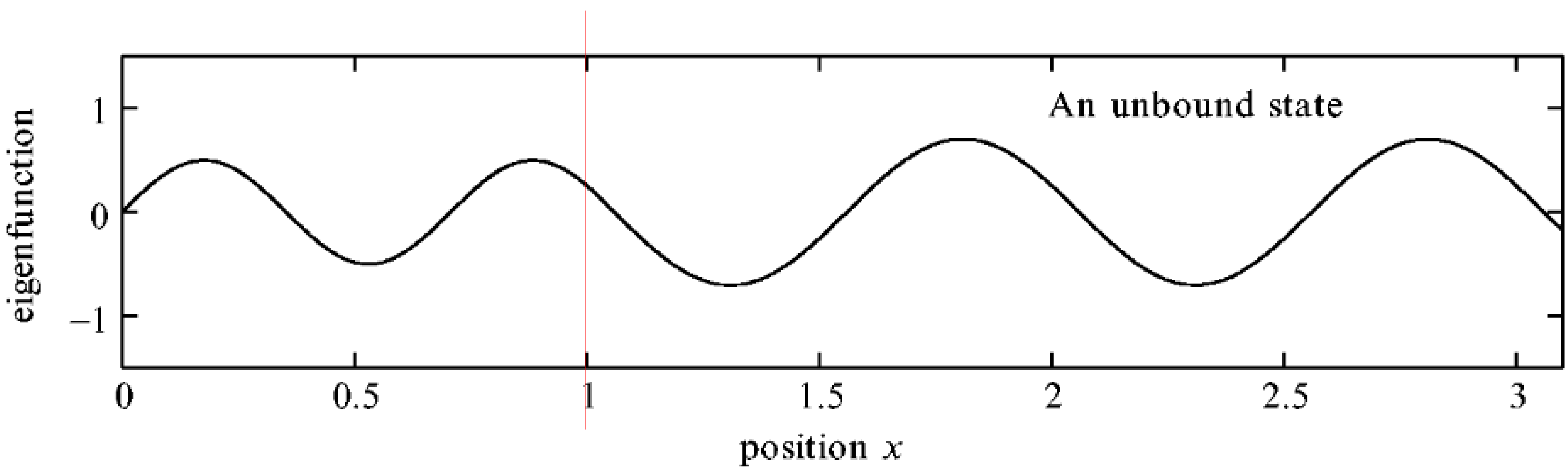
we can write the solutions in the form

wave traveling back and forth inside the well

$$\psi(x) = \begin{cases} A_0\, e^{-ik_0 x} - A_0\, e^{+ik_0 x} & \text{if } 0 < x < a \\ A\, e^{-ikx} - A\, e^{2i\delta}\, e^{+ikx} & \text{if } a < x < \infty. \end{cases}$$

incoming wave

outgoing wave with phase difference 2δ



$a = 1$