PHYS-454

7 - The finite square well

The finite square well-a

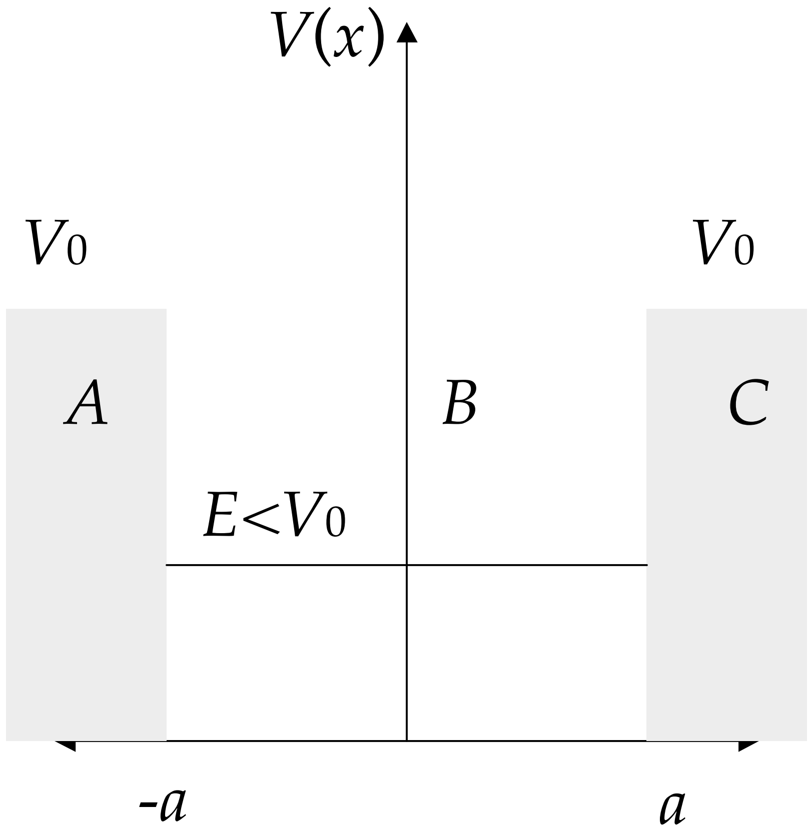
- The finite square well is the next problem that we are going to consider. The solution of Schroedinger equation is not that simple.

The finite square well-b

The potential in this problem has the form:

$$V(x) = \begin{cases} 0 & -a < x < a \\ V_0, & x < -a,\ x > a \end{cases}$$

- Due to the symmetry of the potential the eigenfunctions will be alternatelly even and odd.



Hint: We are looking for bound states in the well. Thus, state for which

$$0<E<V_0$$

Solution of Schroedinger equation

- We can show that the solutions of Schroedinger equation in each of the regions A, B and C are given by:

$$A: \quad \psi''_A + (\varepsilon - U_0)\psi_A = \psi''_A - \gamma^2\psi_A = 0$$

$$B: \quad \psi''_B + \varepsilon\psi_B = \psi''_B + k^2\psi_B = 0$$

$$C: \quad \psi''_C + (\varepsilon - U_0)\psi_C = \psi''_C - \gamma^2\psi_C = 0$$

$$\varepsilon = \frac{2mE}{\hbar^2}, \qquad U_0 = \frac{2mV_0}{\hbar^2}$$

$$\varepsilon = k^2, \quad U_0 - \varepsilon = \gamma^2 \quad (U_0 > \varepsilon)$$

Even solutions-a

In this case the solutions of Schroedinger equations are

$$\psi_A = Ae^{\gamma x}, \quad \psi_B = B\cos kx, \quad \psi_C = Ae^{-\gamma x}$$

Where at region A and C we kept the relevant terms that go to zero at infinity. And we set the coefficients A and C equal in order to satisfy the even character of the solution

$$\psi_A(x) = \psi_C(-x)$$

Even solutions-b

The coefficients A and B are calculated with the help of the following conditions:

$$\psi_B(a) = \psi_C(a) \Rightarrow B\cos\left(ka\right) = Ae^{-\gamma a}$$

$$\psi'_B(a) = \psi'_C(a) \Rightarrow -Bk\sin\left(ka\right) = -\gamma Ae^{-\gamma a}$$

$$\tan\left(ka\right) = \frac{\gamma}{k}$$

Odd solutions-a

In this case the solutions of Schroedinger equations are

$$\psi_A = Ae^{\gamma x}, \quad \psi_B = B\sin kx, \quad \psi_C = -Ae^{-\gamma x}$$

Where at region A and C we kept the relevant terms that go to zero at infinity. And we set the coefficients *C*=-*A* in order to satisfy the odd character of the solution

$$\psi_C(x) = -\psi_A(-x)$$

Odd solutions-b

The coefficients A and B are calculated with the help of the following conditions:

$$\psi_B(a) = \psi_C(a) \Rightarrow B\sin(ka) = -Ae^{-\gamma a}$$

$$\psi'_B(a) = \psi'_C(a) \Rightarrow Bk\cos(ka) = \gamma A e^{-\gamma a}$$

$$\tan(ka) = -\frac{k}{\gamma}$$

Important note: The coefficients A, B and C in the even solutions are different than the ones in the odd solutions! We kept the same symbols for simplicity

Graphical solutions of the eigenvalues-a

- The two equations which they will give us the energy spectrum are:

$$\tan(ka) = \frac{\gamma}{k} \qquad\qquad \tan(ka) = -\frac{k}{\gamma}$$

- This can occur because k and γ depend on energy. But the analytic solution is impossible. We chose a graphical solution.

Graphical solutions of the eigenvalues-b

- We chose a parameter θ related to k and γ by:

$$k = \sqrt{U_0}\cos\theta \qquad \gamma = \sqrt{U_0}\sin\theta$$

Which satisfy the relation $k^2 + \gamma^2 = U_0$

Since k and γ are positive the angle θ is limited in the region $0 \le \theta \le \pi / 2$

Graphical solutions of the eigenvalues-c

- The unknown eigenvalue ε is expressed as a function of the angle θ as follows

$$\varepsilon = U_0 \cos^2\theta \quad \text{or} \quad E = V_0 \cos^2\theta$$

- And our eigenvalues eqs., take the form

$$\tan(ka) = \frac{\gamma}{k} = \tan\theta \qquad \tan(ka) = -\frac{k}{\gamma} = \tan\left(\theta - \frac{\pi}{2}\right)$$

Graphical solutions of the eigenvalues-d

- Solving the above eqs. We get:

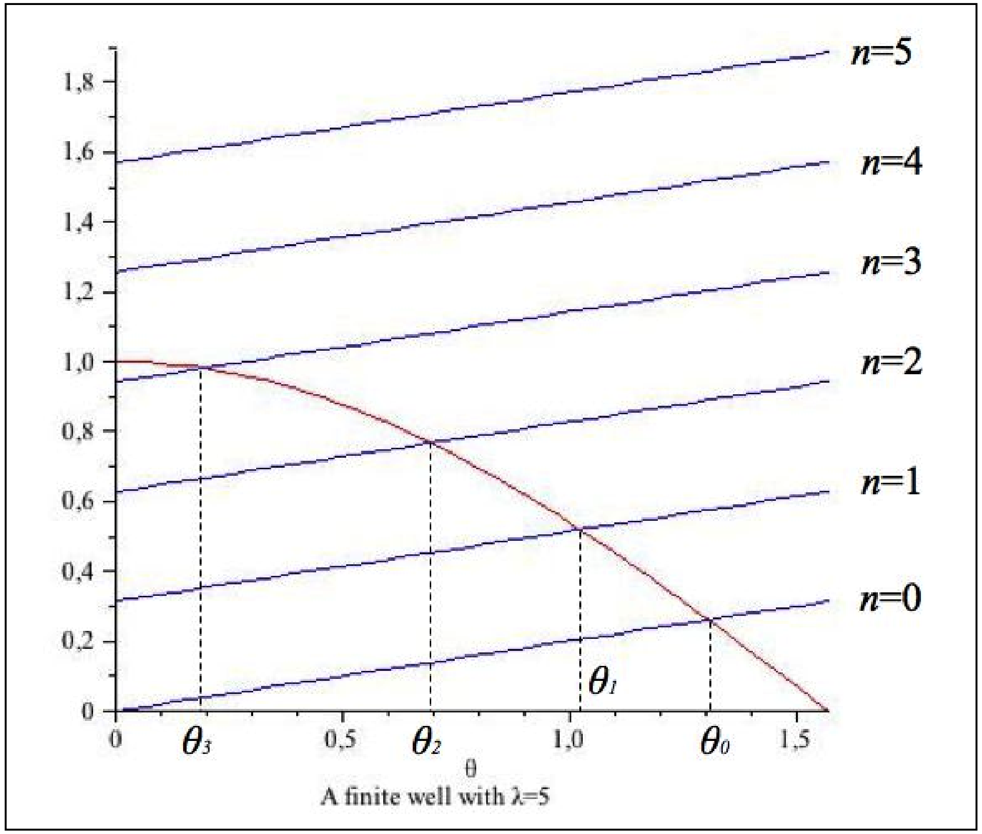
$$\cos\theta = \frac{1}{\lambda}\theta + n\frac{\pi}{2\lambda}, \quad n = 0,\ 1,\ 2,\ 3,\ \ldots, \quad \text{and}\ \ \lambda = a\sqrt{U_0}$$

where even (odd) values for *n* correspond to solutions for even (odd) eigenfunctions.

Graphical solutions of the eigenvalues-e

- The number N of bound states is finite. It is determined from the following relation:

$$N = \left[\frac{\lambda}{\pi / 2} \right] + 1$$

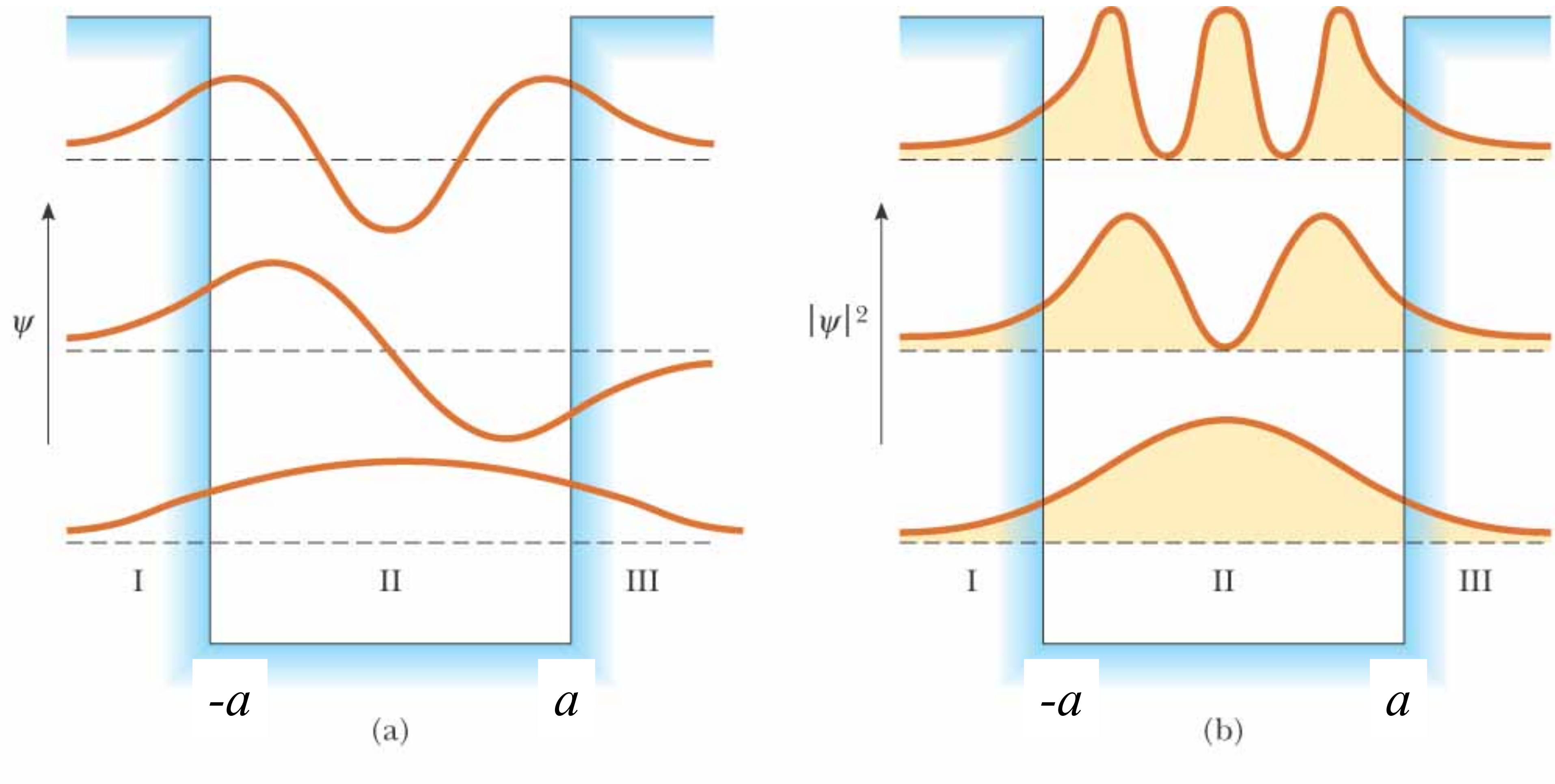


Discussion-a

- The eigenfunctions of the finite square well look like the corresponding ones of the infinite square well, **but**, there is an important difference: *they are not zero at $x=-a$ and $x=a$ but they have exponential "tails" inside the forbiden region.*

x

Discussion-b



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Discussion-c

- We see for first time that a particle can penetrate into a region which is classically forbiden.
- In wave physics we have seen something similar: the electromagnetic waves could penetrate into a conductor where they suffer a damping.
- The fact that the particle can penetrate into this forbiden region gives the wrong impression that in quantum mechanics, sometimes, we can violate the principle of energy conservation.

Discussion-d

- But there is a misconception here: In classical mechanics both kinetic and potential energy can be simultaneously measured and their sum gives always the total energy of the particle.
- In quantum mechanics this is not anymore true: the total energy cannot be separated, at any position, as a sum of a kinetic and a potential term since we cannot measure simultaneously the position and momentum. Thus to say that, at a point x, $E < V(x)$ is *meaningless*.

Discussion-e

- This “paradox” could be also seen in a different way: In the classically forbiden region the wavefunction has an exponential term exp($-\gamma x$). This corresponds to a penetration practically at a length $l=1/\gamma$ (known as penetration length) out of the well.
- If we try to make a measurement and be sure that the particle is out of the well then $\Delta x<l$. But in this case the kinetic energy will be:

Discussion-f

$$\frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2ml^2} = \frac{\hbar^2\gamma^2}{2m} = \frac{\hbar^2}{2m}(U_0 - \varepsilon) = V_0 - E$$

- We see that a measurement which finds the particle in the forbidden region disturbs the energy at least by the amount needed to kick it out of the well!

Discussion-g

- We can see that at the classical limit (very large mass, or very small Planck's constant) the penetration length tends to zero, as it is expected.
- At the strong quantum limit (very small mass or large Planck's constant) it becomes very large!
- *The lighter particles shows strong quantum behaviour!*

$$l = \gamma^{-1} = \sqrt{\frac{\hbar^2}{2m\left(V_0 - E\right)}}$$

Discussion-h

- We can also observe that the deeper the well the smaller the penetration length and vice versa. (As it is expected when the well tends to the infinite depth)
- Also the penetration length depends on the energy. The higher the energy the higher the penetration.