

QUANTUM MECHANICS

Lecture 14

The finite square well:
scattering states

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D. J. Griffiths: paragraph 2.6

Finite potential well: scattering states

Let us come, now, to the stationary solutions corresponding to **scattering states** for the finite square well, for which the (already defined) potential $V(x)$ reads

$$\begin{aligned} |x| \leq a : V(x) &= -V_0 \\ |x| > a : V(x) &= 0 \end{aligned}$$

with $V_0 > 0$.

Finite potential well: scattering states

The scattering solutions correspond to $E > 0$ and, therefore, the equations to be solved are

$$|x| \leq a \quad : \quad -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0\psi = E\psi$$
$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2m(E + V_0)}{\hbar^2}\psi \equiv -r^2\psi$$

$$|x| > a \quad : \quad -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$
$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv -k^2\psi$$

where the coefficients

$$r \equiv \frac{\sqrt{2m(E + V_0)}}{\hbar} \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

are both real and positive.

Finite potential well: scattering states

- 1 The solutions of these second order differential equations are well known:

$$x < -a : \psi(x) = A e^{ikx} + B e^{-ikx}$$

$$|x| \leq a : \psi(x) = C e^{irx} + D e^{-irx}$$

$$x > a : \psi(x) = F e^{ikx} + G e^{-ikx}$$

where the complex constants

A, B, C, D, F, G must guarantee the continuity of ψ and $\psi' \equiv \frac{d\psi}{dx}$ in $\pm a$, together with the normalization of ψ .

- 2 The four continuity conditions will reduce the independent arbitrary constants them from **six to two**.

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Finite potential well: scattering states

- 1 This means that, for every energy $E > 0$ there will be **two** independent solutions.
- 2 Moreover, since $V(x)$ is an **even** function, the **two independent solutions** corresponding to the **same energy** can be chosen to have **opposite parity**.
- 3 However, instead of looking for even/odd solutions, as we have done for the bound states, it is more interesting to look for the so-called **scattering solutions**.

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Finite potential well: scattering states

- 1 By definition, the scattering solutions are such that, in one of the two asymptotic regions, ($x \rightarrow +\infty$ or $x \rightarrow -\infty$) the w.f. consists only of a single phase term:

left – to – right : for $x \rightarrow +\infty$, $\psi(x) \propto e^{ipx}$

right – to – left : for $x \rightarrow -\infty$, $\psi(x) \propto e^{-ipx}$

with $p > 0$.

- 2 In our case, for instance, a left-to-right scattering solution will be characterized by the general structure

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- 2 Let us start by observing that the terms Ae^{ikx} , Be^{-ikx} and Fe^{ikx} contribute to define the wave-function outside the potential region, where the particle is free.

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Finite potential well

Let us remember, now, a general property of the time-dependent Schrödinger equation, concerning the probability.

We have seen that, if we define

$$\begin{aligned}\rho(x, t) &= |\Psi(x, t)|^2 \\ J(x, t) &= -\frac{i\hbar}{2m} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)\end{aligned}$$

then we can write a conservation law as follows

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

Finite potential well

- ① **For a stationary solution**, where $\psi(x, t) = \psi(x, 0)e^{-iEt/\hbar}$
 $|\psi|^2$ and, therefore, ρ cannot be function of time, therefore, in this case, **we have**

$$\frac{dJ}{dx} = 0 \Rightarrow \frac{d}{dx} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right] = 0$$

- ② If we integrate the above equation from any position x_1 to any position x_2 , we obtain

$$\begin{aligned} & \psi^*(x_2) \frac{d\psi}{dx}(x_2) - \psi(x_2) \frac{d\psi^*}{dx}(x_2) = \\ & = \psi^*(x_1) \frac{d\psi}{dx}(x_1) - \psi(x_1) \frac{d\psi^*}{dx}(x_1) \end{aligned}$$

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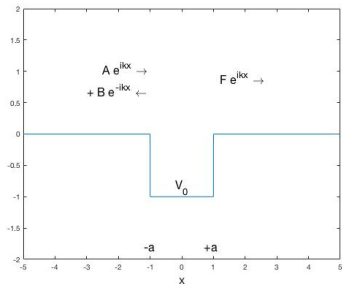
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Finite potential well

Let us apply this general result to our scattering solution and let us assume $x_1 < -a$ and $x_2 > a$. With a straightforward calculation (see next two slides) we obtain

$$|A|^2 - |B|^2 = |F|^2$$



The physical interpretation of the three terms is that Ae^{ikx} describes the incident wave against the potential region, Be^{-ikx} the back-scattered wave (reflected) and Fe^{ikx} the transmitted wave.

calculation ...

We have assumed $x_1 < -a$ and $x_2 > a$: if, for simplicity, we define $\psi_i = \psi(x_i)$, we have

$$\psi_1 = Ae^{ikx_1} + Be^{-ikx_1}; \quad \psi_2 = Fe^{ikx_2}$$

and

$$\begin{aligned} J_2 &\equiv \psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx} = F^* e^{-ikx_2} (ik) F e^{ikx_2} - \\ &- F e^{ikx_2} (-ik) F^* e^{-ikx_2} = 2ik|F|^2 \end{aligned}$$

As far as the term

$$J_1 \equiv \psi_1^* \frac{d\psi_1}{dx} - \psi_1 \frac{d\psi_1^*}{dx}$$

we have

$$\begin{aligned}
 J_1 &= \left(A^* e^{-ikx_1} + B^* e^{ikx_1} \right) ik \left(A e^{ikx_1} - B e^{-ikx_1} \right) - \\
 &- \left(A e^{ikx_1} + B e^{-ikx_1} \right) (-ik) \left(A^* e^{-ikx_1} - B^* e^{ikx_1} \right) = \\
 &= ik \left(|A|^2 - A^* B e^{-2ikx_1} + A B^* e^{2ikx_1} - |B|^2 \right) + \\
 &+ ik \left(|A|^2 - A B^* e^{2ikx_1} + A^* B e^{-2ikx_1} - |B|^2 \right) = \\
 &= 2ik \left(|A|^2 - |B|^2 \right)
 \end{aligned}$$

and, therefore

$$J_1 = J_2 \quad \Rightarrow \quad |A|^2 - |B|^2 = |F|^2$$

Finite potential well

- 1 The explicit evaluation of the coefficients A , B , C , D , F is given in Appendix 4.
- 2 An important quantity, which describes the effect of the potential well on the particle propagation, is the **transmission coefficient** \mathcal{T} defined as

$$\mathcal{T} \equiv \frac{|F|^2}{|A|^2}$$

- 3 From the Appendix calculations, we have

$$F = A e^{-ika} \frac{2kr}{2rk \cos(2ra) - i(r^2 + k^2) \sin(2ra)}$$

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Therefore, we have

$$\begin{aligned}\mathcal{T} &= \frac{4r^2k^2}{4r^2k^2 \cos^2(2ra) + (r^2 + k^2)^2 \sin^2(2ra)} = \\ &= \frac{4r^2k^2}{4r^2k^2 + (r^2 - k^2)^2 \sin^2(2ra)}\end{aligned}$$

The transmission

$$\mathcal{T} = \frac{4r^2k^2}{4r^2k^2 + (r^2 - k^2)^2 \sin^2(2ra)}$$

shows that $\mathcal{T} = 1$ whenever $\sin(2ra) = 0$.

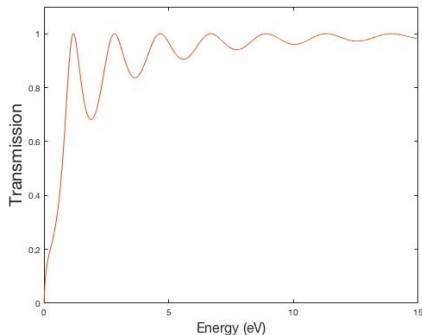
This happens when

$$2ra = n\pi \Rightarrow r \equiv \sqrt{\frac{2m(E + V_0)}{\hbar^2}} = \frac{n\pi}{2a}$$

Finite potential well

Using the definitions of r and k , we obtain

$$\mathcal{T} = \frac{4E(E + V_0)}{4E(E + V_0) + V_0^2 \sin^2(2ra)}$$



The transmission shown in the picture refers to an electron which scatters against a potential well of depth $V_0 = -5 \text{ eV}$ and width $2a = 2 \text{ nm}$.