QUANTUM MECHANICS
Lecture 12

The finite square well (bound states)

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D. J. Griffiths: paragraph 2.6

Bound and scattering states

Until now, we have seen **two different kinds** of wave functions, describing **stationary states** (i.e. solutions of the time-independent Schrödinger equation):

1. **normalizable solutions**, labeled with a discrete index n (infinite square well, harmonic oscillator);
2. **non-normalizable solutions**, labeled by a continuous variable (free particle).

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   - **a sum** (over n) in the first case,
   - **an integral** (over k) in the second case.

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1. Also in Classical Mechanics, a one dimensional time independent potential $V(x)$ can give rise to two different kinds of motion:
   - a bounded trajectory, when $\lim_{x\to\pm\infty} V(x) > E$: in this case, the particle bounces back and forth between the turning points $\hat{x}_{1,2}$ for which $V(\hat{x}) = E$;
   - a trajectory extenting up to infinity, if $E > V(\pm\infty)$: in this case the particle undergo a scattering process.
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2. **The two kinds of solutions of the time independent Schrődinger equation that we have found, correspond precisely to these two situations.**

Bound and scattering states

1. Usually, the potential energy is defined in such a way that it goes to *zero* at $\pm\infty$. In this case, the solutions of the time independent Schrödinger equation describe
   - $E < 0$: **bound states** (normalizable);
   - $E > 0$: **scattering states** (non-normalizable, but with $|\psi|^2$ *limited*...).
2. For the infinite square well and the harmonic oscillator, since $V(\pm\infty) = \infty$, we can have only bound states, whereas for the free particle we can have only scattering states.
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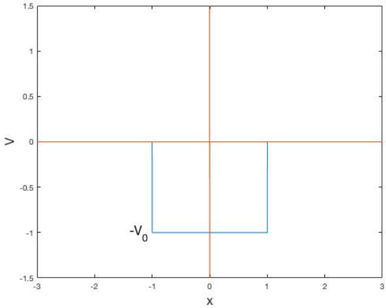
The finite square well

Let us assume that

$$V(x) = 0$$
$$for\, |x| > a$$

$$V(x) = -V_0$$
$$for\, |x| \leq a$$

where V_0 is a suitable **positive** real quantity.



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It is easy to convince ourselves that there are no stationary solutions if $E < -V_0$. In fact

1. from the **mathematical** point of view, it can be shown that it is impossible to fulfill the continuity conditions for ψ and ψ', without having the divergence of $|\psi|^2$ at $+\infty$ or at $-\infty$;

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The finite square well

1. **Let us start by looking for bound states.**
2. Let us assume that $-V_0 < E < 0$.
3. Classically, in this case, the particle would bounce back and forth between $\pm a$.
4. In QM, the time-independent Schrödinger equation for $|x| \leq a$ reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\,\psi$$

$$\Rightarrow \quad \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -(E+V_0)\psi$$

where, by hypothesis, $E + V_0 > 0$.

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

the time-independent Schrödinger equation, for $|x| \leq a$..., becomes

$$\frac{d^2\psi}{dx^2} = -k^2\,\psi$$

2. and its solutions are the well known trigonometric functions

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

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2. Since $E < 0 \;\Rightarrow\; -\frac{2mE}{\hbar^2} \equiv r^2 > 0$ and the solutions are now exponentials

$$\psi(x) = \alpha\, e^{-rx} + \beta\, e^{rx}$$

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Since $|\psi(x)|^2$ must be **square-integrable**,

$$\lim_{x \to \pm\infty} |\psi(x)|^2 = 0$$

we will have

1. even solutions:

$$\begin{aligned} x < -a &\ : \ \alpha\, e^{rx} \\ |x| \leq a &\ : \ B\, cos(kx) \\ x > a &\ : \ \alpha\, e^{-rx} \end{aligned}$$

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1. The continuity of ψ and ψ' for the **even solutions** requires that

$$\begin{aligned} \psi &: \quad \alpha\, e^{-ra} = B\cos(ka) \\ \psi' &: \quad -r\,\alpha\, e^{-ra} = -k\, B\, sin(ka) \end{aligned}$$

2. and therefore that

$$r\, B\cos(ka) = k\, B\, sin(ka) \quad \Rightarrow \quad r = k\, tg(ka)$$

3. with

$$\alpha = B\, e^{ra}\cos(ka)$$

and B to be determined by the normalization condition on $|\psi(x)|^2$.

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1. It is useful, at this point, to define the following two adimensional variables

$$\xi \equiv a\,k = a\sqrt{\frac{2m(E+V_0)}{\hbar^2}} > 0$$

$$\eta \equiv a\,r = a\sqrt{\frac{-2mE}{\hbar^2}} > 0$$

2. In this way, the continuity conditions become

$$even \;:\; r = k\,tg(ka) \;\Rightarrow\; \eta = \xi\,tg\xi$$
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Concerning the constants A and B, defined by the normalization condition on $|\psi|^2$, it can be shown (see Appendix 3) that they are given by:

$$A^{-1} = B^{-1} = \sqrt{a\left(1 + \frac{1}{\eta}\right)}$$

The finite square well

The two adimensional variables ξ and η are such that

$$\begin{aligned} \xi^2 + \eta^2 &= \frac{a^2}{\hbar^2}\left[2m(E+V_0) - 2mE\right] = \\ &= \frac{2mV_0}{\hbar^2} a^2 \equiv R^2 \end{aligned}$$

therefore, the equations to be solved in order to find the possible values of E are

$$\xi^2 + \eta^2 = R^2$$
$$\eta = \xi \, tg\xi \quad or \quad \eta = -\frac{\xi}{tg\xi}$$

and **they can be solved only numerically.**

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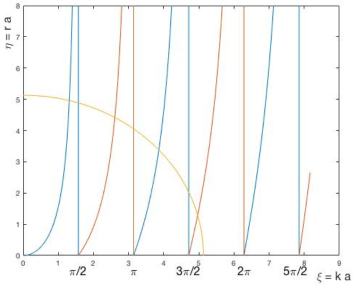

The solutions are alternatively even ($\eta = \xi\, tg\xi$) and odd ($\eta = -\xi\, ctg\xi$). Their total number does not exceed $N = \frac{R}{\pi/2} + 1$.

1. The above example refers to an electron ($mc^2 = 0.511\, MeV$) in a potential well depth of $V_0 = -1\, eV$ and half-width $a = 1\, nm$. Since $\hbar c = 197\, Mev \cdot fm$, the value of R is $R = 5.2$ and there are only four possible bound states ($\frac{5.2}{\pi/2} + 1 = 4.31$).

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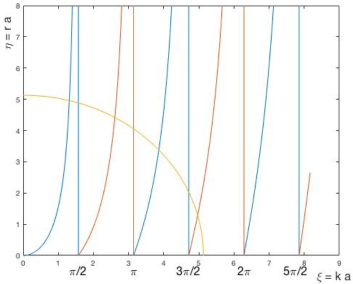

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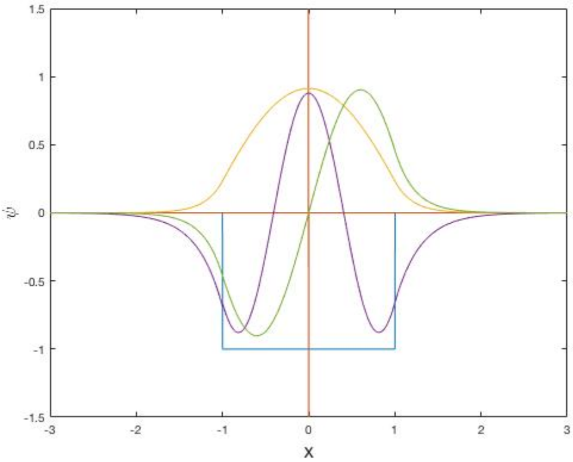
The first three (not-normalized) stationary solutions ...



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1. Let us remark,now, an important difference with respect to what we have found for the infinite square well.

2. The p.d.f. $|\psi(x)|^2$ associated to the stationary (bound) states is different from zero also in the region outside the well, where the total energy is smaller that the potential energy.

3. This region is forbidden in Classical Mechanics !

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