QUANTUM MECHANICS
Lecture 7
The infinite square well

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September 24, 2019

D. J. Griffiths: paragraph 2.2

The infinite square well

1. **Let us start, now, to solve our first time-independent Schrődinger equation !**

2. Assume a potential energy $V(x)$ such that

$$\begin{aligned} V(x) &= 0 \quad if \quad 0 \leq x \leq a \\ V(x) &= +\infty \quad otherwise \end{aligned}$$

This corresponds to a situation where the particle is free in the region $0 \leq x \leq a$, but, at the two ends of the region ($x = 0$ and $x = a$), there is an infinite force that prevents the particle to escape outside from the well.

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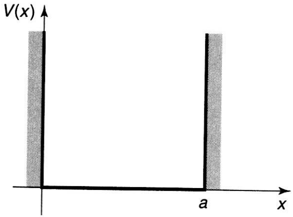

We can, therefore, assume that $\Psi(x,t) = 0$ when $x < 0$ or when $x > a$, because the probability to find the particle outside the well has to be zero.

1. Inside the well, the time-independent Schrödinger equation reads

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

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = -k^2\,\psi \quad with \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

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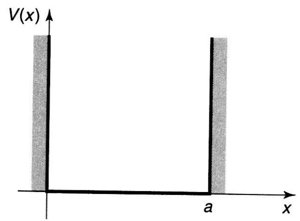

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1. We have here implicitly assumed that $E > 0$ on a physical basis, since, in this region, the total energy coincides with the kinetic energy which is always positive.

2. From the mathematical point of view, the case $E < 0$ would give rise to solutions which are exponentials with a real argument and it would be impossible to fulfill the w.f. continuity conditions at $x = 0$ and $x = a$, requiring that $\psi(0) = \psi(a) = 0$.

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The equation that we have obtained

$$\frac{d^2\psi}{dx^2} = -k^2\,\psi \quad with \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

is the classical equation of a harmonic oscillator: its well known solutions are

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

with A and B arbitrary integration constants, to be determined with the help of the boundary conditions, defined by the continuity of ψ at $x = 0$ and $x = a$.

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1. The ψ continuity at $x = 0$ implies that $B = 0$, which means that that

$$\psi(x) = A\, sin\, kx$$

whereas the ψ continuity at $x = a$ requires that

$$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \ldots$$

2. The value $k = 0$ must be escluded, since it will imply that $\psi(x) = 0$ everywhere, and the negative k do not add any new solution, because they correspond to solutions with k positive and $A \rightarrow -A$.

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1. Therefore, the only possible values for k are the following ones

$$k = \frac{n\pi}{a} \quad with \quad n = 1,\, 2,\, 3, \ldots$$

2. and the solutions of the time-independent Schrödinger equation for the infinite potential well are, therefore, the following

$$\psi_n(x) = A\, sin\left(\frac{n\pi x}{a}\right); \quad n = 1,\, 2,\, 3, \ldots$$

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The energy associated to the ψ_n is defined by the time-independent Schrödinger equation itself: we have

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\,\frac{d^2\psi_n}{dx^2} &= E_n\,\psi_n \\
\Rightarrow \quad E_n &= \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2
\end{aligned}
$$

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As far as the constant A, as we already know, due to the linear structure of the Schrödinger equation, it is **arbitrary.**

However, if we require the ψ_n to be **normalized** and **real**, then ($\phi \equiv \frac{n\pi x}{a}$)

$$
\begin{aligned}
1 &= \int dx\ |\psi_n(x)|^2 = A^2 \int_0^a dx\, sin^2\left(\frac{n\pi x}{a}\right) = \\
&= A^2\, \frac{a}{n\pi} \int_0^{n\pi} d\phi\ sin^2\phi = \\
&= A^2\, \frac{a}{n\pi} \int_0^{n\pi} d\phi\ \frac{1}{2}(1 - cos2\phi) = \\
&= A^2\, \frac{a}{n\pi}\, \frac{n\pi}{2} = A^2\, \frac{a}{2} \quad \Rightarrow \quad A = \sqrt{\frac{2}{a}}
\end{aligned}
$$

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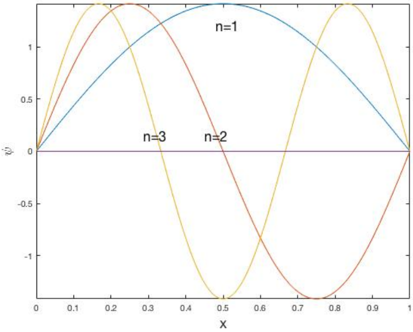
In conclusion, the normalized *time − independent* solutions of the Schrödinger equation for the infinite square well can be written as



$$\psi_n(x) = \sqrt{\frac{2}{a}}\, sin\left(\frac{n\pi x}{a}\right); \quad n = 1,\, 2,\, \ldots$$

The infinite square well

1. The wave function ψ_1 corresponds to the **ground state**, the physical state of minimal energy, and the other functions ψ_n with $n > 1$ correspond to **excited states.**
2. The ψ_n are alternately even and odd with respect to the center of the well.
3. The number of nodes (zeroes) of ψ_n is $n - 1$.

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1. The ψ_n, as we have shown in a previous lecture, are mutually orthogonal, which means that, being normalized, they are orthonormal:

$$\int dx\ \psi_r^*(x)\,\psi_s(x) = \delta_{rs}$$

where δ_{rs} is the Kronecker symbol:
when both indices are equal its value is 1, otherwise is 0.

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The infinite square well

1. The functions ψ_n are an **orthonormal** and **complete** set of functions in the domain $0 \leq x \leq a$.

2. As a matter of fact, any continuous function $f(x)$ such that $f(0) = f(a) = 0$ can be written in the segment $[0, a]$ as a linear combination of them:

$$f(x) = \sum_n c_n \, \psi_n(x)$$

which is nothing but the **Fourier expansion.**

3. Because of the orthonormality of the ψ_n, the expansion coefficients c_n are simply given by

$$c_n = \int dx \; \psi_n^*(x) \cdot f(x)$$

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This means that, the most **general solution** of the **time – dependent** Schrödinger equation reads

$$\Psi(x,t) = \sum_n c_n \sqrt{\frac{2}{a}}\, sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar}$$

where

$$\begin{aligned} E_n &= \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{1}{2m}\left(\frac{n\pi\hbar}{a}\right)^2 \\ c_n &= \int dx\ \psi_n^*(x)\,\Psi(x,0) \end{aligned}$$

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1. **There is any physical meaning in the expansion coefficients c_n ?**
2. Let us start by observing that

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In fact, from the normalization of the w.f. Ψ, we have$^{(*)}$

$$
\begin{aligned}
1 &= \int dx\, |\Psi(x,0)|^2 = \\
&= \int dx \left(\sum_r c_r \psi_r(x) \right)^* \left(\sum_s c_s \psi_s(x) \right) = \\
&= \sum_{r,s} c_r^* c_s \int dx\, \psi_r^*(x) \psi_s(x) = \\
&= \sum_{r,s} c_r^* c_s\, \delta_{rs} = \sum_r |c_r|^2
\end{aligned}
$$

(*) Why it is enough to consider the normalization condition at $t = 0$?

The infinite square well

Moreover, it turns out that the **energy expectation value** (constant in time !) is given by

$$< H >= \sum_s E_s \, |c_s|^2$$

In fact

$$< H >= \int dx \, \Psi^*(x,t) \left[\hat{H} \, \Psi(x,t) \right] =$$

$$= \int dx \left(\sum_r c_r \psi_r e^{-iE_r t/\hbar} \right)^* \left[\hat{H} \left(\sum_s c_s \psi_s e^{-iE_s t/\hbar} \right) \right] =$$

$$= \sum_{r,s} c_r^* \, c_s \, e^{i(E_r - E_s)t/\hbar} \, E_s \int dx \, \psi_r^* \, \psi_s =$$

$$= \sum_s |c_s|^2 \, E_s$$

The infinite square well

1. From these two results, it is easy to understand **the physical meaning** of the expansion coefficients $\mathbf{c_n}$.

2. The quantity $|\mathbf{c_n}|^2$ gives **the probability** that a measurement of the total energy on the physical state under consideration **would yield the value** E_n.

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Exercise N.3

Evaluate the expectation values $< x >$ and $< p >$, together with the standard deviations σ_x and σ_p on the first excited state, represented by the w.f. $\Psi_2(x,t)$

$$\psi_2(x) = \sqrt{\frac{2}{a}}\, sin\left(\frac{2\pi x}{a}\right) \quad for \quad 0 \leq x \leq a$$

and verify the uncertainty relation.