Introduction to Quantum Physics

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Abstract

The video channel with the title "Professor M does Science" in YouTube offers a simple step-by-step but all the same very valuable and rigorous introduction into the world of quantum physics. This script covers the calculus of wave functions and helps to digest the topic covered by a group of those videos but is not meant as a replacement for them.

3 The Calculus of Wave Functions in Quantum Mechanics

3.1 Wave Functions

A wave function is one of the possible ways to look at a quantum system. It is the so-called position representation of quantum mechanics. This representation is useful when examining system is the three-dimensional space including potential barriers.

The position operator $\hat{x}$ with the eigenvalue equation $\hat{x}\,|x\rangle = x\,|x\rangle$ and the momentum operator $\hat{p}$ with the eigenvalue equation $\hat{p}\,|p\rangle = p\,|p\rangle$ satisfy the commutation relation $[\hat{x}, \hat{p}] = i\,\hbar$. The position eigenstates $|x\rangle$ form an orthonormal basis such that $\langle x|x'\rangle = \delta(x - x')$, and any state can therefore be represented as $|\psi\rangle = \int dx\ \langle x|\psi\rangle\,|x\rangle$. The *wave function* is defined as $\psi(x) = \langle x|\psi\rangle$ in the basis of the eigenstates of the position operator. Wave functions are fundamental in quantum mechanics and form the formulation called wave mechanics. Similarly, the momentum eigenstates $|p\rangle$ form an orthonormal basis such that $\langle p|p'\rangle = \delta(p - p')$, and any state can therefore be represented as $|\psi\rangle = \int dp\ \langle p|\psi\rangle\,|p\rangle$. The wave function in momentum space is $\bar{\psi}(p) = \langle p|\psi\rangle$.

The scalar product of $|\psi\rangle = \int dx\ \langle x|\psi\rangle\,|x\rangle$ and $|\varphi\rangle = \int dy\ \langle y|\varphi\rangle\,|y\rangle$ is

$$\begin{aligned}\langle\psi|\varphi\rangle &= \left(\int dx\ \langle\psi|x\rangle\,|x\rangle\right)\left(\int dy\ \langle y|\varphi\rangle\,|y\rangle\right) = \int dx \int dy\ \langle\psi|x\rangle\,\langle y|\varphi\rangle\,\langle x|y\rangle \\ &= \int dx \int dy\,\psi^*(x)\,\varphi(y)\,\delta(x-y) = \int dx\,\psi^*(x)\,\varphi(x)\end{aligned}$$

and this is the usual scalar product between two wave functions but has been developed from the scalar product for states. The norm is

$$\langle\psi|\psi\rangle = \int dx\,\psi^*(x)\,\psi(x) = \int dx\,|\psi(x)|^2$$

and a wave function $\psi(x)$ is normalized if $\langle\psi|\psi\rangle = 1$. Scalar product and norm are similarly defined in momentum space for a wave function $\bar{\psi}(p)$.

Switching from the representation in position space with basis $\{|x\rangle\}$ to the representation in momentum space with basis $\{|p\rangle\}$ is done using the overlap matrix $\langle x|p\rangle$. The translation operator is needed in the form for an infinitesimal amount ε

$$\hat{T}(-\varepsilon) = e^{i\,\varepsilon\,\hat{p}/\hbar} = \mathbb{I} + \frac{i\,\varepsilon}{\hbar}\hat{p} + O(\varepsilon^2)$$

together with the properties $\hat{T}(\alpha)\,|x\rangle = |x+\alpha\rangle$ and $\langle x|\,\hat{T}(\alpha) = \langle x-\alpha|$. The derivation

$$\begin{aligned}\langle x+\varepsilon|p\rangle &= \langle x|\hat{T}(-\varepsilon)|p\rangle = \langle x|\left(\mathbb{I} + \frac{i\,\varepsilon}{\hbar}\hat{p} + O(\varepsilon^2)\right)|p\rangle = \langle x|p\rangle + \frac{i\,\varepsilon}{\hbar}\,\langle x|\hat{p}|p\rangle + O(\varepsilon^2)\\ &= \langle x|p\rangle + \frac{i\,\varepsilon}{\hbar}p\,\langle x|p\rangle + O(\varepsilon^2)\end{aligned}$$

leads to

$$p\,\langle x|p\rangle = -i\,\hbar\lim_{\varepsilon\to 0}\left(\frac{\langle x+\varepsilon|p\rangle - \langle x|p\rangle}{\varepsilon}\right) = -i\,\hbar\frac{d}{dx}\,\langle x|p\rangle \qquad \Rightarrow \qquad \frac{d\,\langle x|p\rangle}{\langle x|p\rangle} = \frac{i}{\hbar}p\,dx$$

and $\ln(\langle x|p\rangle) = \frac{i}{\hbar}\,p\,x + c$ and further by integration to

$$\langle x|p\rangle = N\,e^{i\,p\,x/\hbar}$$

where $N = e^c$ still has to be determined. Using $\langle x|x'\rangle = \delta(x-x')$ in

$$\begin{aligned}\langle x|x'\rangle &= \langle x|\mathbb{I}|x'\rangle = \langle x|\left(\int dp\ |p\rangle\langle p|\right)|x'\rangle = \int dp\ \langle x|p\rangle\,\langle p|x'\rangle = |N|^2\int dp\,e^{i\,p\,(x-x')/\hbar}\\ &= |N|^2\,2\pi\,\hbar\,\delta(x-x') = \delta(x-x')\end{aligned}$$

and using one of the possible definitions of a delta function

$$\delta(x-x') = \frac{1}{2\pi}\int du\,e^{i\,u(x-x')}$$

with $u = p/\hbar$ gives $|N|^2 = \frac{1}{2\pi\,\hbar}$ and therefore

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\,\hbar}}\,e^{i\,p\,x/\hbar}$$

is the scalar product of an eigenstate in position space and an eigenstate in momentum space. Again inserting $\mathbb{I}$ into $\langle p|\psi\rangle = \bar{\psi}(p)$ and similarly in the other direction leads to

$$\bar{\psi}(p) = \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\,\hbar}}\int dx\,e^{-i\,p\,x/\hbar}\,\psi(x) \qquad \psi(x) = \langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\,\hbar}}\int dp\,e^{i\,p\,x/\hbar}\,\bar{\psi}(p) \tag{3.1}$$

showing that switching from position space to momentum space and vice versa uses the *Fourier transform*.

In three dimensions with $\underline{\hat{x}} = (\hat{x}_1,\hat{x}_2,\hat{x}_3)$ and $\underline{\hat{p}} = (\hat{p}_1,\hat{p}_2,\hat{p}_3)$ the commutation relations generalize to $[\hat{x}_j,\hat{p}_k] = i\,\hbar\,\delta_{jk}$. The eigenvalue equation can be written as $\underline{\hat{x}}\,|\underline{x}\rangle = \underline{x}\,|\underline{x}\rangle$ and the other equations can be adapted similarly. The Fourier transform generalizes to

$$\psi(\underline{x}) = \frac{1}{(2\pi\,\hbar)^{3/2}}\int d\underline{p}\,e^{i\,\underline{p}\cdot\underline{x}/\hbar}\,\bar{\psi}(\underline{p})$$

and analogously for $\bar{\psi}(\underline{p})$.

Wave functions are therefore simply a particular representation in the more general framework of state vectors. Wave mechanics can be embedded into quantum mechanics in a state space, and wave functions are states in the continuous basis of position or momentum.

3.2 Action of the Position and Momentum Operator on Wave Functions

The position operator $\hat{x}$ acts by multiplying the wave function by x and the momentum operator $\hat{p}$ acts on the wave function by calculating the derivative. This is shown here.

Using the fact that $\langle x|\psi\rangle = \psi(x)$ is the wave function and that the action of $\hat{x}$ on $|\psi\rangle$ gives another state $\hat{x}\,|\psi\rangle = |\psi'\rangle$ together with the eigenvalue equation $\hat{x}\,|x\rangle = x\,|x\rangle$ gives

$$\psi'(x) = \langle x|\psi'\rangle = \langle x|\hat{x}|\psi\rangle = x\,\langle x|\psi\rangle = x\,\psi(x)$$

and this implies that the action of the position operator in terms of wave functions is simply multiplication by x. Similarly, for $|\psi'\rangle = \hat{p}\,|\psi\rangle$ is

$$\bar{\psi}'(p) = \langle p|\psi'\rangle = \langle p|\hat{p}|\psi\rangle = p\,\langle p|\psi\rangle = p\,\bar{\psi}(p)$$

the action of the momentum operator. Thus, the action of the position operator in its own basis is very simple, and the action of the momentum operator in its own basis is also very simple.

The action of the momentum operator in the position basis and vice versa is harder. With $\langle x|\psi\rangle = \psi(x)$ and $|\psi'\rangle = \hat{p}\,|\psi\rangle$ the value of $\langle x|\hat{p}|\psi\rangle$ has to be determined. To do so one can start from the translation operator to get

$$\begin{aligned}\psi(x+\varepsilon) = \langle x+\varepsilon|\psi\rangle = \langle x|\hat{T}(-\varepsilon)|\psi\rangle = \langle x|\left(\mathbb{I} + \frac{i\,\varepsilon}{\hbar}\hat{p} + O(\varepsilon^2)\right)|\psi\rangle = \langle x|\psi\rangle + \frac{i\,\varepsilon}{\hbar}\,\langle x|\hat{p}|\psi\rangle + O(\varepsilon^2)\\ = \psi(x) + \frac{i\,\varepsilon}{\hbar}\,\langle x|\hat{p}|\psi\rangle + O(\varepsilon^2)\end{aligned}$$

and to get further

$$\langle x|\hat{p}|\psi\rangle = -i\,\hbar \lim_{\varepsilon\to 0}\left(\frac{\psi(x+\varepsilon)-\psi(x)}{\varepsilon}\right) = -i\,\hbar\,\frac{d\psi(x)}{dx}$$

showing that the action of the momentum operator $\hat{p}$ on $|\psi\rangle$ when written in the position representation means a derivative on the wave function multiplied by $-i\,\hbar$.

To get the action of the position operator in the momentum basis one can use the Fourier transformation (3.1) and start from $|\psi'\rangle = \hat{x}\,|\psi\rangle$ with

$$\bar{\psi}'(p) = \langle p|\psi'\rangle \qquad \bar{\psi}(p) = \langle p|\psi\rangle \qquad \psi'(x) = \langle x|\psi'\rangle \qquad \psi(x) = \langle x|\psi\rangle$$

to get

$$\bar{\psi}'(p) = \frac{1}{\sqrt{2\pi\,\hbar}}\int dx\, e^{-i\,p\,x/\hbar}\,\psi'(x) = \frac{1}{\sqrt{2\pi\,\hbar}}\int dx\, e^{-i\,p\,x/\hbar}\,x\,\psi(x)$$

using $\psi'(x) = x\,\psi(x)$ from above. Because of

$$\frac{d}{dp}\left(e^{-i\,p\,x/\hbar}\,\psi(x)\right) = -\frac{i\,x}{\hbar}e^{-i\,p\,x/\hbar}$$

one can write

$$\bar{\psi}'(p) = i\,\hbar\,\frac{d}{dp}\left[\frac{1}{\sqrt{2\pi\,\hbar}}\int dx\, e^{-i\,p\,x/\hbar}\,\psi(x)\right] = i\,\hbar\,\frac{d\bar{\psi}(p)}{dp}$$

showing that the action of the position operator in the momentum basis is the derivative times $i\,\hbar$.

These results can be transferred to the three-dimensional space. In the position representation on one hand where the wave function is $\psi(\underline{x}) = \langle\underline{x}|\psi\rangle$, the position operator $\hat{\underline{x}}$ simply multiplies the wave function by $\underline{x}$ giving $\underline{x}\,\psi(\underline{x})$ and the momentum operator $\hat{\underline{p}}$ acts as $-i\,\hbar\,\nabla_{\underline{x}}\,\psi(\underline{x})$. In the momentum representation where $\bar{\psi}(p) = \langle\underline{p}|\psi\rangle$, the action of the position operator $\hat{\underline{x}}$ calculates the gradient $\nabla_{\underline{p}}$ with respect to $\underline{p}$ as $i\,\hbar\,\nabla_{\underline{p}}\,\bar{\psi}(p)$, and the momentum operator $\hat{\underline{p}}$ simply multiplies the wave function by $\underline{p}$.

3.3 Parity Operator

The parity operator describes the reflection about the origin. In one dimensions, for example, it reflects a wave function $\psi(x)$ to $\psi(\text{-}x)$. Therefore, it is also called the space inversion operator. It is useful in problems with inversion symmetry such as the infinite square well. From the fundamental interactions the electromagnetic and the strong nuclear force are symmetric under parity. Only the weak nuclear force breaks parity.

The *parity operator* $\hat{\pi}$ acts on a position eigenstate $|\underline{x}\rangle$ as $\hat{\pi}\,|\underline{x}\rangle = |\text{-}\underline{x}\rangle$. Given this definition the action of the parity operator can be extended to any state represented in the position representation. The parity operator acting on a momentum eigenstate $|\underline{p}\rangle$, for example, gives

$$\hat{\pi}\,|\underline{p}\rangle = \hat{\pi}\left(\frac{1}{(2\pi\,\hbar)^{3/2}}\int d\underline{x}\, e^{i\,\underline{p}\cdot\underline{x}/\hbar}\,|\underline{x}\rangle\right) = \frac{1}{(2\pi\,\hbar)^{3/2}}\int d\underline{x}\, e^{i\,\underline{p}\cdot\underline{x}/\hbar}\,\hat{\pi}\,|\underline{x}\rangle = \frac{1}{(2\pi\,\hbar)^{3/2}}\int d\underline{x}'\, e^{i\,(-\underline{p})\cdot\underline{x}'/\hbar}\,|\underline{x}'\rangle$$
$$= |\text{-}\underline{p}\rangle$$

where $\underline{x}' = \text{-}\underline{x}$. Note that $\int d(\text{-}\underline{x}') = \int d\underline{x}'$ because of integration over the whole space. This shows that the parity operator acts on position and momentum eigenstates in the same way. It simple reflects both quantities about the origin.

In order to determine the action of the parity operator on an arbitrary state $|\psi\rangle$ the state is represented in the position representation as

$$|\psi\rangle = \int d\underline{x}\,\psi(\underline{x})\,|\underline{x}\rangle$$

where $\psi(\underline{x}) = \langle\underline{x}|\psi\rangle$ is the wave function. The action of the parity operator is

$$\hat{\pi}\,|\psi\rangle = \hat{\pi}\int d\underline{x}\,\psi(\underline{x})\,|\underline{x}\rangle = \int d\underline{x}\,\psi(\underline{x})\hat{\pi}\,|\underline{x}\rangle = \int d\underline{x}\,\psi(\underline{x})\,|\text{-}\underline{x}\rangle$$

and it is convenient to see what this new state looks like

$$\langle\underline{x}|\hat{\pi}|\psi\rangle = \langle\underline{x}|\int d\underline{x}'\,\psi(\underline{x}')|\text{-}\underline{x}'\rangle = \int d\underline{x}'\,\psi(\underline{x}')\,\langle\underline{x}\,|\text{-}\underline{x}'\rangle = \int d\underline{x}'\,\psi(\underline{x}')\delta(\underline{x} - (\text{-}\underline{x}')) = \psi(\text{-}\underline{x})$$

in the position representation. Thus, the parity operator reflects the wave function about the origin. The same is true in the momentum representation.

The parity operator is involutory $\hat{\pi} = \hat{\pi}^{-1}$ because $\hat{\pi}^2\,|\underline{x}\rangle = |\underline{x}\rangle \Rightarrow \hat{\pi}^2 = \mathbb{I}$, and it is also Hermitian $\hat{\pi} = \hat{\pi}^\dagger$ because its definition $\hat{\pi}\,|\underline{x}\rangle = |\text{-}\underline{x}\rangle$ is $\langle\underline{x}|\,\hat{\pi}^\dagger = \langle\text{-}\underline{x}|$ in dual space and

$$\langle\underline{y}|\hat{\pi}|\underline{x}\rangle = \langle\underline{y}|\text{-}\underline{x}\rangle = \delta(\underline{y} - (\text{-}\underline{x})) = \delta(\underline{x} + \underline{y}) \qquad\qquad \langle\underline{y}|\hat{\pi}^\dagger|\underline{x}\rangle = \langle\text{-}\underline{y}|\underline{x}\rangle = \delta(\text{-}\underline{y} - \underline{x}) = \delta(\underline{x} + \underline{y})$$

using the fact that the delta function is an even function. It follows that it is also unitary $\hat{\pi}^{-1} = \hat{\pi}^\dagger$.

The eigenvalues and eigenstates follow from the eigenvalue equation $\hat{\pi}\,|\lambda\rangle = \lambda\,|\lambda\rangle$ and $\hat{\pi}^2 = \mathbb{I}$ with

$$|\lambda\rangle = \mathbb{I}\,|\lambda\rangle = \hat{\pi}^2\,|\lambda\rangle = \lambda\hat{\pi}\,|\lambda\rangle = \lambda^2\,|\lambda\rangle$$

such that $\lambda^2 = 1$ and $\lambda = \pm 1$. This was to be expected because the eigenvalues of Hermitian operators are real numbers and the eigenvalues of unitary operators satisfy $|\lambda|^2 = 1$. The eigenstate associated with $\lambda = +1$ is called $|\psi_+\rangle$ and the eigenstate associated with $\lambda = -1$ is called $|\psi_-\rangle$ such that the eigenvalue equation for the parity operator becomes $\hat{\pi}\,|\psi_\pm\rangle = \pm\,|\psi_\pm\rangle$. The eigenstate $|\psi_+\rangle$ is called even, and the eigenstate $|\psi_-\rangle$ is called odd, and even or odd states are said to have definite parity. The position and momentum eigenstates do not satisfy the eigenvalue equation of the parity operator and are therefore not eigenstates.

In terms of wave functions this eigenvalue equation means

$$\begin{aligned} &\hat{\pi}\,|\psi_+\rangle = +\,|\psi_+\rangle &&\Rightarrow \langle\underline{x}|\hat{\pi}|\psi_+\rangle = +\,\langle\underline{x}|\psi_+\rangle &&\Rightarrow \psi_+(\text{-}\underline{x}) = +\psi_+(\underline{x}) \\ &\hat{\pi}\,|\psi_-\rangle = -\,|\psi_-\rangle &&\Rightarrow \langle\underline{x}|\hat{\pi}|\psi_-\rangle = -\,\langle\underline{x}|\psi_-\rangle &&\Rightarrow \psi_-(\text{-}\underline{x}) = -\psi_-(\underline{x}) \end{aligned}$$

and the even eigenstates give even wave functions $\psi_+(\text{-}\underline{x}) = +\psi_+(\underline{x})$ while odd eigenstates give odd wave functions $\psi_-(\text{-}\underline{x}) = -\psi_-(\underline{x})$.

To show that the two operators $\hat{P}_+ = \frac{1}{2}(\mathbb{I} + \hat{\pi})$ and $\hat{P}_- = \frac{1}{2}(\mathbb{I} - \hat{\pi})$ are projection operators one has to show that they are idempotent. This follows from

$$\begin{aligned} \hat{P}_+^2 &= \frac{1}{4}(\mathbb{I} + \hat{\pi})(\mathbb{I} + \hat{\pi}) = \frac{1}{4}(\mathbb{I} + \hat{\pi} + \hat{\pi} + \hat{\pi}^2) = \frac{1}{2}(\mathbb{I} + \hat{\pi}) = \hat{P}_+ \\ \hat{P}_-^2 &= \frac{1}{4}(\mathbb{I} - \hat{\pi})(\mathbb{I} - \hat{\pi}) = \frac{1}{4}(\mathbb{I} - \hat{\pi} - \hat{\pi} + \hat{\pi}^2) = \frac{1}{2}(\mathbb{I} - \hat{\pi}) = \hat{P}_- \end{aligned}$$

using the fact that $\hat{\pi}^2 = \mathbb{I}$. The product $\hat{P}_+\hat{P}_-$ is

$$\hat{P}_+\hat{P}_- = \frac{1}{4}(\mathbb{I}+\hat{\pi})(\mathbb{I}-\hat{\pi}) = \frac{1}{4}(\mathbb{I}+\hat{\pi}-\hat{\pi}-\hat{\pi}^2) = 0$$

showing that these two operators project on orthogonal subspaces. Further, the sum of the two operators due to

$$\hat{P}_+ + \hat{P}_- = \frac{1}{2}(\mathbb{I}+\hat{\pi}) + \frac{1}{2}(\mathbb{I}-\hat{\pi}) = \mathbb{I}$$

project on complementary subspaces. These two operators project onto eigenstates of the parity operator as

$$\hat{\pi}(\hat{P}_+ |\psi\rangle) = \hat{\pi}\frac{1}{2}(\mathbb{I}+\hat{\pi})|\psi\rangle = \frac{1}{2}(\hat{\pi}+\hat{\pi}^2)|\psi\rangle = \frac{1}{2}(\hat{\pi}+\mathbb{I})|\psi\rangle = \hat{P}_+|\psi\rangle \qquad \Rightarrow \hat{P}_+|\psi\rangle = |\psi_+\rangle$$
$$\hat{\pi}(\hat{P}_- |\psi\rangle) = \hat{\pi}\frac{1}{2}(\mathbb{I}-\hat{\pi})|\psi\rangle = \frac{1}{2}(\hat{\pi}-\hat{\pi}^2)|\psi\rangle = \frac{1}{2}(\hat{\pi}-\mathbb{I})|\psi\rangle = \text{-}\hat{P}_-|\psi\rangle \qquad \Rightarrow \hat{P}_-|\psi\rangle = |\psi_-\rangle$$

proves. Finally, any state $|\psi\rangle$ can be written as the sum of an even and an odd state as

$$|\psi\rangle = \mathbb{I}|\psi\rangle = (\hat{P}_+ + \hat{P}_-)|\psi\rangle = \hat{P}_+|\psi\rangle + \hat{P}_-|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle$$

shows.

3.4 Even and Odd Operators

Even operators are the operators that commute with the parity operator, and odd operators anticommute with the parity operator. Since many Hamiltonians are even the eigenstates for an even Hamiltonian must be even or odd states, and this fact simplifies many calculations.

An even operator $\hat{A}_+$ is defined by $[\hat{A}_+, \hat{\pi}] = 0$. An equivalent alternative definition for an even operator is $\hat{A}_+ = \hat{\pi}\hat{A}_+\hat{\pi}$ as

$$\hat{A}_+\hat{\pi} = \hat{\pi}\hat{A}_+ \Rightarrow \hat{A}_+\hat{\pi}^2 = \hat{\pi}\hat{A}_+\hat{\pi} \Rightarrow \hat{A}_+\mathbb{I} = \hat{A}_+ = \hat{\pi}\hat{A}_+\hat{\pi}$$

proves. This shows the unitary transformation of $\hat{A}_+$ and this means that an even operator is one that does not change under the unitary operator provided by the parity operator.

Because even operators commute with the parity operator it is always possible to find a common set of eigenstates for these two operators. This means that the eigenstates of an even operator are either even or odd states. More formally, from the eigenvalue equation $\hat{A}_+|\lambda\rangle = \lambda|\lambda\rangle$ with $|\lambda_\pm\rangle = \hat{P}_\pm|\lambda\rangle$ such that $\hat{\pi}|\lambda_\pm\rangle = \pm|\lambda_\pm\rangle$ and $[\hat{A}_+, \hat{P}_\pm] = [\hat{A}_+, \frac{1}{2}(\mathbb{I}\pm\hat{\pi})] = 0$ follows

$$\hat{A}_+|\lambda_\pm\rangle = \hat{A}_+\hat{P}_\pm|\lambda\rangle = \hat{P}_\pm\hat{A}_+|\lambda\rangle = \lambda\hat{P}_\pm|\lambda\rangle = \lambda|\lambda_\pm\rangle$$

assuming that λ is non-degenerate. Thus, the parity eigenstates are also eigenstates of $\hat{A}_+$, and the eigenvalue in this case is λ. The eigenstates of an even operator have a definite parity. In the case of degenerate eigenvalues, it is always possible to apply a transformation in this degenerate subspace to obtain a new set of eigenstates that are also eigenstates of the parity operator as shown above for compatible observables.

An odd operator $\hat{A}_-$ is defined by $\{\hat{A}_-, \hat{\pi}\} = 0$. An equivalent alternative definition for an odd operator is $\hat{A}_- = -\hat{\pi}\hat{A}_-\hat{\pi}$ as

$$\hat{A}_-\hat{\pi} = -\hat{\pi}\hat{A}_- \Rightarrow \hat{A}_-\hat{\pi}^2 = -\hat{\pi}\hat{A}_-\hat{\pi} \Rightarrow \hat{A}_-\mathbb{I} = \hat{A}_- = -\hat{\pi}\hat{A}_-\hat{\pi}$$

proves. Because odd operators do not commute with the parity operator they do not generally share a common set of eigenstates. This means that other than in the case of even operators the eigenstates of odd operators do not have a definite parity.

So far, the terms "even" and "odd" have been introduced for states and for operators. However, one should not confuse these terms. Thus, to summarize, even operators are defined by $[\hat{A}_+, \hat{\pi}] = 0$ and their eigenstates are also eigenstates of the parity operator and are therefore either even or odd states. Odd operators are defined by $\{\hat{A}_-, \hat{\pi}\} = 0$ and their eigenstates have no definite parity.

Many important physical systems have operators that are powers of even or odd operators. Thus, the parity properties of powers of operators are needed. In the case of even operators using $\mathbb{I} = \hat{\pi}^2$

$$\hat{\pi}\hat{A}_+^n\hat{\pi} = \hat{\pi}\hat{A}_+\mathbb{I}\hat{A}_+\mathbb{I}...\mathbb{I}\hat{A}_+\hat{\pi} = \hat{\pi}\hat{A}_+\hat{\pi}\hat{\pi}\hat{A}_+\hat{\pi}\hat{\pi}...\hat{\pi}\hat{\pi}\hat{A}_+\hat{\pi} = \hat{A}_+^n$$

shows $\hat{A}_+^n = \hat{\pi}\hat{A}_+^n\hat{\pi}$ and $\hat{A}_+^n$ is therefore also an even operator. For odd operators a similar calculation

$$\hat{\pi}\hat{A}_-^n\hat{\pi} = \hat{\pi}\hat{A}_-\mathbb{I}\hat{A}_-\mathbb{I}...\mathbb{I}\hat{A}_-\hat{\pi} = \hat{\pi}\hat{A}_-\hat{\pi}\hat{\pi}\hat{A}_-\hat{\pi}\hat{\pi}...\hat{\pi}\hat{\pi}\hat{A}_-\hat{\pi} = (\text{-}1)^n\hat{A}_-^n$$

shows that $\hat{A}_-^n$ is an odd operator for n odd and an even operator for n even.

A general function $F(\hat{A})$ can be written in form of a power series as shown above. A function $F(\hat{A}_+)$ of an even operator gives therefore also an even operator. The situation for functions of odd operators is a bit more difficult because their power series usually contain even and odd powers. Thus, a function $F(\hat{A}_-)$ of an odd operator has generally no definite parity. However, there are two special cases. If $F(-x) = F(x)$ as a function of real numbers, then $F(\hat{A}_-)$ is an even operator, and its power series contains only even powers of $\hat{A}_-$. Similarly, if $F(-x) = -F(x)$ as a function of real numbers, then $F(\hat{A}_-)$ is an odd operator, and its power series contains only odd powers of $\hat{A}_-$.

Many operators in quantum mechanics happen to be either even or odd operators. The position operator $\underline{\hat{r}} = (\hat{x}, \hat{y}, \hat{z})$ with the eigenvalue equation $\hat{x}\,|x\rangle = x\,|x\rangle$ as an example component is an odd operator as

$$\hat{\pi}\hat{x}\,|x\rangle = x\hat{\pi}\,|x\rangle = x\,|\text{-}x\rangle \quad \hat{x}\hat{\pi}\,|x\rangle = \hat{x}\,|\text{-}x\rangle = \text{-}x\,|\text{-}x\rangle \quad \Rightarrow (\hat{\pi}\hat{x} + \hat{x}\hat{\pi})\,|x\rangle = \{\hat{x}, \hat{\pi}\}\,|x\rangle = 0 \quad \Rightarrow \{\hat{x}, \hat{\pi}\} = 0$$

proves since $|x\rangle$ is an arbitrary basis state. The same argument for $\hat{y}$ and $\hat{z}$ shows that $\{\underline{\hat{r}}, \hat{\pi}\} = 0$. The momentum operator satisfies $\{\underline{\hat{p}}, \hat{\pi}\} = 0$ and is therefore also an odd operator.

More important are the even operators because they have definite parity. A very important operator is the Hamiltonian $\hat{H}$ as it describes a physical system. It consists of two terms

$$\hat{H} = \frac{\underline{\hat{p}}^2}{2m} + V(\underline{\hat{r}})$$

where the kinetic energy is an even operator because it is an even power of an odd operator and the potential energy is just a function of an odd operator without a definite parity. Thus, the Hamiltonian in this general form has no definite parity. However, for even potentials the Hamiltonian is an even operator. Examples of even potentials are the infinite square well potential and the quantum harmonic oscillator both discussed below. The harmonic oscillator has the quadratic potential $V(x) = \frac{1}{2}m\omega^2x^2$, and that is an even function in x. Also the hydrogen atom has an even potential.

3.5 Infinite Square Well Potential

One of the most iconic problems in quantum mechanics is the one-dimensional infinite square well potential. The infinite square well potential describes a particle in a box. There are two reasons why this problem is interesting. Firstly it is one of the few problems that can be solved exactly in quantum mechanics, and secondly many more complicated problems such as electrons in atoms are essentially electrons trapped in a potential well.

The Hamiltonian with the kinetic and the potential energie and the time independent Schrödinger equation as its eigenvalue equation are

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad \hat{H}\psi(x) = E\psi(x) \qquad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

where $\psi(x)$ is a wave function. The potential $V(x)$ for the infinite square well is

$$V(x) = \begin{cases} 0 & \text{for } |x| < \frac{a}{2} \\ \infty & \text{for } |x| > \frac{a}{2} \end{cases}$$

such that there are impenetrable walls at $\pm\frac{a}{2}$. Thus, the wave function $\psi(x)$ must

(i) vanish outside where the potential is infinite such that $\psi(x) = 0$ for $|x| > \frac{a}{2}$
(ii) be continuous such that $\psi(x) = 0$ for $x = \pm\frac{a}{2}$
(iii) be determined mathematically for $|x| < \frac{a}{2}$

and the equation to be solved for the solution inside the well is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

because the potential is zero.

This is a second order linear differential equation and one can always try the solution $e^{i\,k\,x}$ with the 2nd derivation $\frac{d^2}{dx^2}(e^{i\,k\,x}) = -k^2 e^{i\,k\,x}$. Inserting this into the eigenvalue equation gives

$$-\frac{h^2}{2m}\left(-k^2\,e^{i\,k\,x}\right) = E\,e^{i\,k\,x} \qquad \Rightarrow k^2 = \frac{2m\,E}{\hbar^2} \qquad \Rightarrow k = \begin{cases} +\frac{\sqrt{2m\,E}}{\hbar} & = +k \\ -\frac{\sqrt{2m\,E}}{\hbar} & = -k \end{cases}$$

and the general solution together with the energy eigenvalues are

$$\psi(x) = A\,e^{i\,k\,x} + B\,e^{-i\,k\,x} \qquad E = \frac{\hbar^2\,k^2}{2m}$$

with $A, B \in \mathbb{C}$.

To go from the general solution to the specific solution of the problem one has to include the boundary conditions. This gives

$$\begin{aligned} \psi\Big(+\frac{a}{2}\Big) &= 0 \qquad \Rightarrow A\,e^{i\,k\,a/2} + B\,e^{-i\,k\,a/2} = 0 \qquad \Rightarrow A = -B\,e^{-i\,k\,a} \\ \psi\Big(-\frac{a}{2}\Big) &= 0 \qquad \Rightarrow A\,e^{-i\,k\,a/2} + B\,e^{i\,k\,a/2} = 0 \qquad \Rightarrow A = -B\,e^{i\,k\,a} \end{aligned}$$

such that $e^{-i\,k\,a} = e^{i\,k\,a}$ and therefore $1 = e^{i\,2\pi\,n} = e^{2i\,k\,a}$ for $n \in \mathbb{Z}$. Thus, k is $k_n = \frac{\pi\,n}{a}$ and can only be a multiple of $\frac{\pi}{a}$. The solution to the problem of this well potential is an oscillation, and only oscillations where the number of oscillations exactly fit the well are solutions. Because the energy depends on k also the energy can only take discrete values such that

$$E_n = \frac{\hbar^2\,k_n^2}{2m} = \frac{\hbar^2\,\pi^2\,n^2}{2m\,a^2} = \varepsilon\,n^2 \tag{3.2}$$

for $n \in \mathbb{Z}$.

To get the wave functions the complex numbers A and B are needed and can be determined as

$$A = -B\,e^{i\,k\,a} = -B\,e^{i\,\pi\,n} = (-1)^{n+1}B = \begin{cases} +B & \text{for odd } n \\ -B & \text{for even } n \end{cases}$$

and the wave function becomes

$$\psi(x) = \begin{cases} A\,e^{i\,k\,x} + A\,e^{-i\,k\,x} = 2A\,\cos(k\,x) = 2A\,\cos\left(\frac{\pi\,n\,x}{a}\right) & \text{for odd } n \\ A\,e^{i\,k\,x} - A\,e^{-i\,k\,x} = 2iA\,\sin(k\,x) = 2iA\,\sin\left(\frac{\pi\,n\,x}{a}\right) & \text{for even } n \end{cases}$$

for the still unknown A. This value can be determined since $\psi(x)$ has to be normalized. This leads for odd n to

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = 4|A|^2 \int_{-a/2}^{+a/2} \cos^2\left(\frac{\pi\,n\,x}{a}\right)\,dx = 4|A|^2 \int_{-a/2}^{+a/2} \frac{1}{2}\left(1 + \cos\left(\frac{2\pi\,n\,x}{a}\right)\right)\,dx \\ &= 2|A|^2\left(\Big[x\Big]_{-a/2}^{+a/2} + \frac{a}{2\pi\,n}\left[\sin\left(\frac{2\pi\,n\,x}{a}\right)\right]_{-a/2}^{+a/2}\right) = 2|A|^2\Big[x\Big]_{-a/2}^{+a/2} = 2|A|^2\,a \end{aligned}$$

with integration inside the well only because the wave function vanishes outside the well. Thus, $|A|^2 = \frac{1}{2a}$, and the phase choice $A = \frac{1}{\sqrt{2a}}$ makes A a real number.

The similar calculation for even n

$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx$$

gives the same result $|A|^2 = \frac{1}{2a}$ but the phase choice sets $A = -\frac{i}{\sqrt{2a}}$ here such that $2iA$ becomes real, and the final wave function becomes

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos\left(\frac{\pi \, n \, x}{a}\right) & \text{for odd } n \\ \sqrt{\frac{2}{a}} \sin\left(\frac{\pi \, n \, x}{a}\right) & \text{for even } n \end{cases} \tag{3.3}$$

where it is obvious that the eigenstates of the Hamiltonian have definite parity because the coordinates have been chosen such that $[\hat{H}, \hat{\pi}] = 0$. The eigenstates $\psi_n(x)$ for $n = 1, ..., 6$ is shown in figure 1.

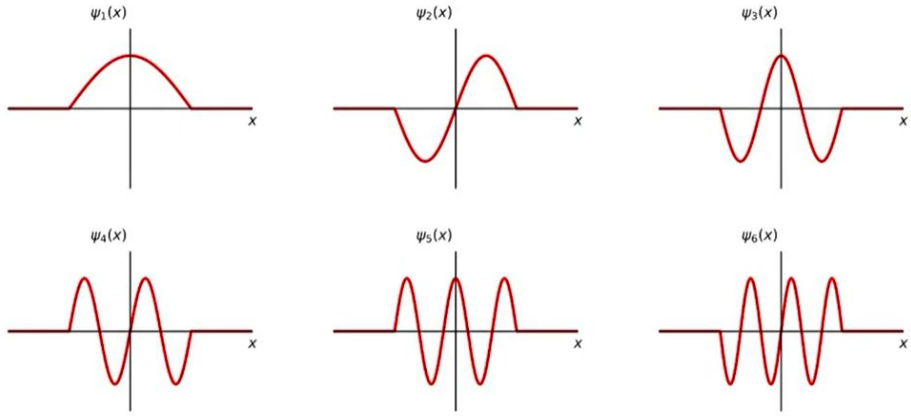


Figure 1: The first six eigenstates for the infinite square well potential

The energy eigenvalues E_n in (3.2) have been written as $E_n = \varepsilon \, n^2$ where ε is a constant. The energy levels for $n = 1, 2, 3, ...$ are $E_1 = \varepsilon$, $E_2 = 4\,\varepsilon$ and $E_3 = 9\,\varepsilon$ and so on, and the jumps from E_n to E_{n+1} become bigger and bigger because of the factor n^2.

3.6 Time Evolution After a Quantum Measurement

The dynamics of a quantum system is governed by the Schrödinger equation

$$i\,\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + V(x)\,\psi(x,t)$$

which is here written in the position representation for the one-dimensional case. When the potential $V(x)$ is independent of time then the dynamics of the system takes a particularly simple form. The system at time $t = 0$ is $\psi(x,0) = \sum_n c_n(0)\psi_n(x)$ for the eigenstates $\hat{H}\psi_n(x) = E_n\psi_n(x)$ of the Hamiltonian, and the system at time $t > 0$ is $\psi(x,t) = \sum_n c_n(t)\psi_n(x)$ where $c_n(t) = c_n(0)\, e^{-i\,E_n\,t/\hbar}$. If the state is an eigenstate of the Hamiltonian then only a single term appears in the sum and the time dependence becomes trivial because $\psi(x,t) = c_j(t)\,\psi_j(x) = c(0)\,e^{-i\,E_n\,t/\hbar}\,\psi_j(x)$. The relevant information about the system is given by $|\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t) = |c_j(0)|^2 |\psi_j(x)|^2$ where the time dependent exponents vanished, and these states are called stationary states because they are time independent.

If there is more than one non-zero term in this sum for $\psi(x,t)$ then one can follow the steps

(1) solve the eigenvalue equation $\hat{H}\psi_n(x) = E_n\psi_n(x)$ to get E_n and $\psi_n(x)$
(2) expand $\psi(x,0)$ in the basis $\{\psi_n(x)\}$ of eigenstates
(3) construct $\psi(x,t)$ by building the coefficients $\{c_n(t)\}$

and this recipe is in the following applied to the infinite square well potential discussed above. For the first step the eigenvalues and eigenstates have been determined and are shown in (3.2) and (3.3).

To show the time evolution the superposition of two energy eigenstates

$$\psi(x,0) = \frac{1}{\sqrt{2}} \left(\psi_j(x) + \psi_k(x)\right) \qquad\qquad c_j(0) = c_k(0) = \frac{1}{\sqrt{2}}$$

is used as the initial wave function. The wave function at time t is

$$\psi(x,t) = \frac{1}{\sqrt{2}} \left(\psi_j(x)\, e^{-i\, E_j\, t/\hbar} + \psi_k(x)\, e^{-i\, E_k\, t/\hbar}\right)$$

and to get $|\psi(x,t)|^2$ one can multiply $\psi(x,t)$ by a global phase

$$e^{i\, E_j\, t/\hbar}\psi(x,t) = \frac{1}{\sqrt{2}} \left(\psi_j(x) + \psi_k(x)\, e^{-i\,(E_k - E_j)\, t/\hbar}\right)$$

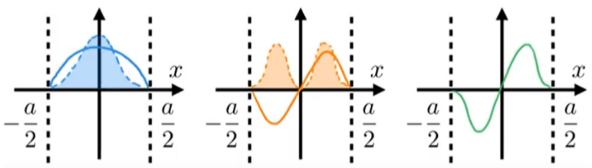
isolating the time dependence in one term. Thus,

$$\begin{aligned} |\psi(x,t)|^2 &= \psi^*(x,t)\, \psi(x,t) \\ &= \frac{1}{2} \left(|\psi_j(x)|^2 + |\psi_k(x)|^2 + \psi_j^*(x)\, \psi_k(x)\, e^{-i\,(E_k - E_j)\, t/\hbar} + \psi_k^*(x)\, \psi_j(x)\, e^{i\,(E_k - E_j)\, t/\hbar}\right) \end{aligned}$$

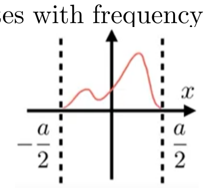
has four terms where the first two are time independent and the cross-terms capture the time dependence. Because $\psi_n(t) \in \mathbb{R}$ such that $\psi_n^*(t) = \psi_n(t)$ the cross-terms can be combined and

$$|\psi(x,t)|^2 = \frac{1}{2} \left(|\psi_j(x)|^2 + |\psi_k(x)|^2 + 2\, \psi_j(x)\, \psi_k(x)\, \cos\left(\frac{(E_k - E_j)t}{\hbar}\right)\right)$$

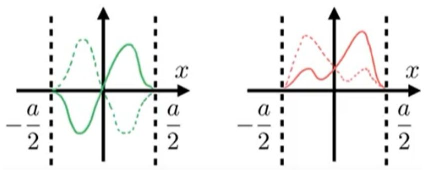
has only one time dependent cross-term. The frequency at which the cosine oscillates is given by the energy difference $(E_k - E_j)/\hbar$. The cross-term is called the mixing term, and it allows more interesting dynamics than those of the stationary states.



The figure on the left side shows the three terms $|\psi_1(x)|^2$, $|\psi_2(x)|^2$, $2\psi_1(x)\psi_2(x)$ where $\psi_1(x)$ and $\psi_2(x)$ are also drawn in the first two graphs and the third graph illustrates the cross-term at $t = 0$. The third graph actually oscillates with frequency $\omega = (E_k - E_j)/\hbar$.

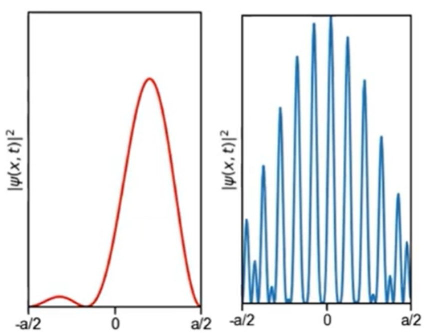


If one adds the three terms together one gets the graph in the figure on the right side. This shows the situation at $2\pi n/\omega$ for $n \in \mathbb{Z}$ because the period of $2\psi_1(x)\psi_2(x)\cos(\omega t)$ is $T = 2\pi/\omega$.



One can get an impression of the oscillation by looking at the cross-term and the sum for $t = \frac{1}{2}T$ as illustrated in the figure on the left side. The first two terms are time independent and stay therefore the same and the cross-term together with the sum are mirrored about the vertical axis corresponding to the middle of the well leading to the dashed lines. The high peak on the right side of the sum has decreased in size and the small peak on the left side has increased in size. A smooth change in time makes the two peaks therefore oscillate at a frequency ω.

The illustration on the right side shows two cases of a superposition $\frac{1}{\sqrt{2}}(\psi_j(x) + \psi_k(x))$. The left graph with $j = 1$ and $k = 2$ as in the above graphics is compared with the right graph with $j = 1$ and $k = 20$. Because of $\omega \propto E_k - E_j$ and $E_n \propto n^2$ the energy of the oscillation in the right graph is much higher than the energy of the oscillation in the left graph.



From the system that mixes two energy levels one can now look at the more general problem of a mixture of many energy levels by examining the time evolution after a position measurement. The position measurement collapses the wave function to a single point in space where the particle is measured to be. Thus, the initial wave function is $\psi(x,0) = \delta(x - x_0)$ where x_0 is the position in space where the particle has been measured to be. However, the delta function is not normalizable, and it is not a valid wave function belonging to the Hilbert space. Thus, saying that the particle is at x_0 means that it is in a small region centered at x_0. One writes $\Delta(x - x_0)$ which is a function that peaks at x_0 but has a finite width. This makes the function normalizable and therefore a proper wave function in the Hilbert space.

Still using the delta function gives

$$\psi(x,0) = \sum_n c_n(0)\,\psi_n(x) \qquad c_n(0) = \int_{-\infty}^{+\infty} \psi_n(x)\psi(x,0)dx = \int_{-\infty}^{+\infty} \psi_n(x)\delta(x - x_0)\,dx = \psi_n(x_0)$$

for the initial wave function and

$$\psi(x,t) = \sum_n c_n(0)\, e^{-i\,E_n\,t/\hbar}\,\psi_n(x) = \sum_n \psi_n(x_0)\, e^{-i\,E_n\,t/\hbar}\,\psi_n(x)$$

for the wave function evolving in time where $\psi_n(x_0)$ is a constant and $\psi_n(x)$ is a function of x. To replace $\psi(x,0) = \delta(x - x_0)$ by $\Delta(x - x_0)$ all one has to do from a numerical point of view is to truncate the sum over n to some finite number of terms. This gives a properly normalizable wave function. The reason why one obtains a finite width by truncating the sum is that there is no longer the destructive interference working in the case of the delta function.

Because at a time $t_1 > 0$ each basis function oscillates at a different frequency $\omega_n = E_n/\hbar$, this will break further the destructive interference that led to the very localized wave function at the beginning. This means that the probability distribution of the overall wave function will spread. At much later times t_∞ the initial coherence to localize the state at a single point will be completely destroyed, and the probability distribution for the wave function will become more or less flat.

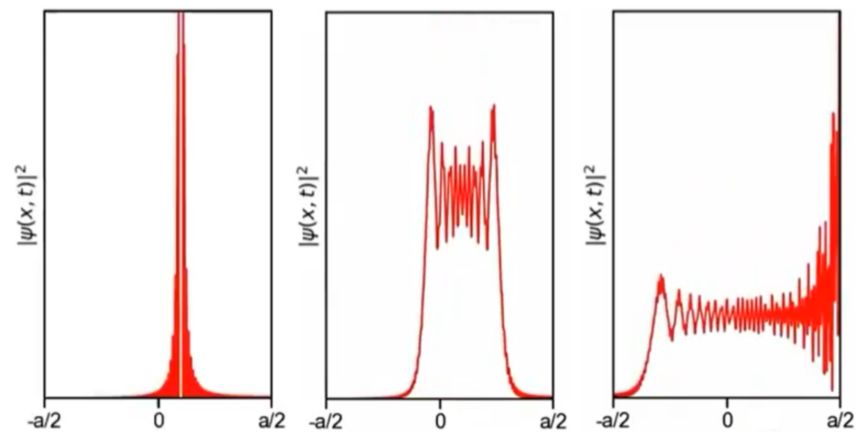


Figure 2: Three $|\psi(x,t_j)|^2$ for wave function with $t_0 < t_1 < t_2$ for the infinite square well

The three graphs in figure 2 illustrate the time evolution of the probability distribution for the overall wave function $\psi(x,t)$. At time $t_0 = 0$ the initial probability distribution for $\psi(x,0) = \Delta(x - x_0)$ shown in the left graph is centered at x_0 and is very narrow. At a later time t_1 the probability distribution in the middle starts spreading and gets wider, and at time t_2 in the graph on the right side the probability distribution hits the right wall. In the end at $t = \infty$ the particle can be anywhere in the well and the probability distribution is completely flat.

Comparing classical mechanics with quantum mechanics shows the difference clearly. At $t = 0$ the particle is exactly at x_0 classically but is only around $x_0 \approx \Delta(x - x_0)$ in quantum mechanics. At $t > 0$ Newton's laws tell that the particle is exactly at $x(t)$ in classical physics while time evolution is governed by Schrödinger's equation in quantum mechanics and gives only the wave function $\psi(x,t)$ stating the probability $P(x,t)dx = |\psi(x,t)|^2 dx$ of the particle being in $(x, x + dx)$ at time t if one measures it again.