Considerations related to the Dirac δ-function.

Related information you may find at:

https://www.reed.edu/physics/faculty/wheeler/documents/Miscellaneous%20Math/Delta%20Functions/Simplified%20Dirac%20Delta.pdf

Griffiths, 3.3 Eigenfunctions of a Hermitian Operator

Hope I can help you with learning quantum mechanics.

Contents

Eigenvalue and eigenfunction

The X-operator applied to a function $f(x)$ delivers $xf(x)$:

$$(Xf)(x) = xf(x)$$

In quantum mechanics there should be eigenvalues and eigenfunctions:

$$(Xf)(x) = \lambda f(x) \rightarrow xf(x) = \lambda f(x)$$

With ordinary functions this is not possible. We extend the space of continuous functions by the Dirac δ-function.

Extending $\mathbb{Q}$

Using rational numbers, we can build the equation $x \cdot x = 4$ with the solution $x = 2$. This works with every square number on the right side. In contrast $x \cdot x = 2$ has no solution within the rational numbers. What we can do is building sequences that match better and better with the real solution:

$$1 \cdot 1 = 1 < 2 < 2 \cdot 2 = 4$$

$$1.4 \cdot 1.4 = 1.96 < 2 < 1.5 \cdot 1.5 = 2.25$$

$$1.41 \cdot 1.41 = 1.9881 < 2 < 1.42 \cdot 1.42 = 2.0164$$

These sequences converge. The converging point is not a rational number.

What we do is: we give these converging sequences a new Symbol: $\sqrt{2}$

With this we can solve the equation:

$$x \cdot x = 2 \rightarrow x = \sqrt{2}$$

Meaning: we can build a sequence of rational numbers that match the desired value to a precision needed. We extend the set of rational numbers $\mathbb{Q}$ by these symbols and build a new set, the set of real numbers $\mathbb{R}$.

Square integrable functions

In quantum mechanics we need functions that are square integrable, meaning:

$$\int_{-\infty}^{\infty} f(x)dx = c$$

Note: c is an existing number, $c \neq \infty$

The X-operator applied to a function:

$$(Xf)(x) = xf(x)$$

For an operator we have the eigenvalue property:

$$(Xf)(x) = \lambda f(x)$$

Note: λ is eigenvalue, $f(x)$ is eigenfunction.

A possible solution:

$$f_\lambda(x) = \begin{cases} 0 \; for \; x \neq \lambda \\ c \; for \; x = \lambda \end{cases}$$

Note: c is a constant.

This function fulfills the eigenvalue property:

$$x \cdot f_\lambda(x) =$$

$$x \cdot \begin{cases} 0 \; for \; x \neq \lambda \\ c \; for \; x = \lambda \end{cases} =$$

$$\begin{cases} 0 \; for \; x \neq \lambda \\ \lambda \cdot c \; for \; x = \lambda \end{cases} =$$

$$\lambda \cdot \begin{cases} 0 \; for \; x \neq \lambda \\ c \; for \; x = \lambda \end{cases} =$$

$$\lambda \cdot f_\lambda(x)$$

The problem is the scalar product. With an arbitrary function $g(x)$ we get:

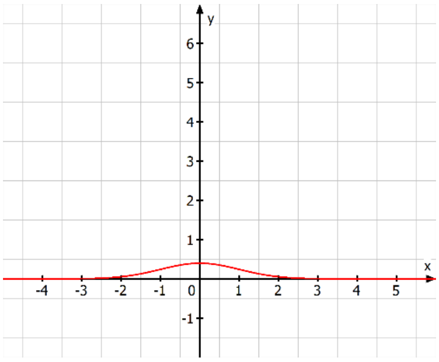
$$\int_{-\infty}^{\infty} f_\lambda(x) g(x) dx = 0$$

$f_\lambda(x)$ is not suitable for use with the scalar product.

The Dirac δ-function

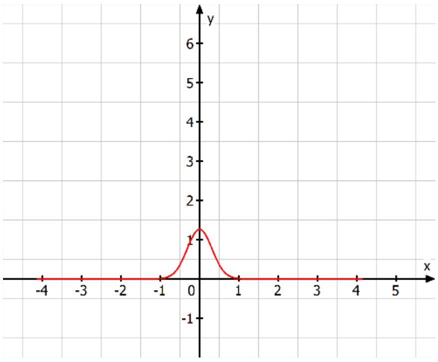
We build a sequence of the following functions:

$$f_n(x) = \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot x^2\right)$$

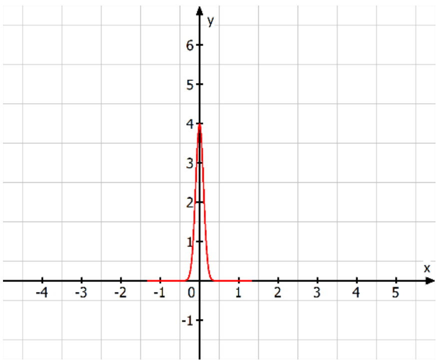


$n = 1$

...



$n = 10$



$n = 100$

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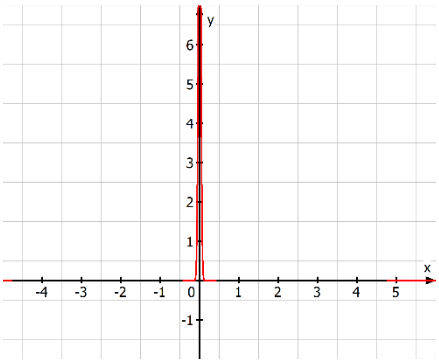


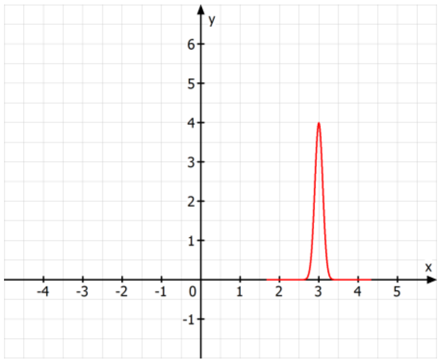
$n = 1000$

The area below the function remains 1:

$$\sqrt{\frac{n}{2\pi}} \cdot \int_{-\infty}^{\infty} \exp\left(-\frac{n}{2} \cdot x^2\right) dx = \sqrt{\frac{n}{2\pi}} \cdot \sqrt{\frac{\pi}{\frac{n}{2}}} = 1$$

We can shift the function on the x-axis by changing the argument to $(x - x_0)$:

$$f_{n,x_0}(x) = \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x - x_0)^2\right)$$



$n = 100, x_0 = 3$

We try the scalar product with the function $g(x) \coloneqq 5$. We use the formula:

$$\int_{-\infty}^{\infty} \exp(-(ax^2 - bx + c))dx = \sqrt{\frac{\pi}{a}} \cdot e^{\left(\frac{b^2}{4a} - c\right)}$$

$g(x) \coloneqq 5$	$g(x) \coloneqq 5$
$\int_{-\infty}^{\infty} f_1(x)g(x)dx =$ $\int_{-\infty}^{\infty} \sqrt{\frac{1}{2\pi}} \cdot \exp\left(-\frac{1}{2} \cdot (x-3)^2\right) \cdot 5dx =$ $\sqrt{\frac{25}{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2} \cdot (x-3)^2\right) dx =$ $\sqrt{\frac{25}{2\pi}} \cdot \sqrt{2\pi} = 5$	$\int_{-\infty}^{\infty} f_{10}(x)g(x)dx =$ $\int_{-\infty}^{\infty} \sqrt{\frac{10}{2\pi}} \cdot \exp\left(-\frac{10}{2} \cdot (x-3)^2\right) \cdot 5dx =$ $\sqrt{\frac{250}{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{10}{2} \cdot (x-3)^2\right) dx =$ $\sqrt{\frac{250}{2\pi}} \cdot \sqrt{\frac{\pi}{5}} = 5$

This seems to work.

If we take the limes $n \to \infty$:

$$f_{n,x_0}(x) = \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x - x_0)^2\right)$$

we get the Dirac δ-function:

$$\delta_{x_0}(x) = \lim_{n \to \infty} \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x - x_0)^2\right)$$

The Dirac δ-function $\delta_{x_0}(x)$ performs what we need with respect to the eigenvalue/eigenvector problem:

$$x \cdot \delta_{x_0}(x) = x_0 \cdot \delta_{x_0}(x)$$

We replace x_0 with λ and write:

$$x \cdot \delta_\lambda(x) = \lambda \cdot \delta_\lambda(x)$$

Note: the Dirac δ-function has no existing value at position x_0. This is similar to the case in which we extended rational numbers by square roots. The square root $\sqrt{2}$ cannot be represented by a natural number or by a fraction of natural numbers – it is the limes of a sequence of fractions. The same holds for the Dirac δ-function.

The Dirac δ-function applied to polynomials

We restrict to polynomials and check the monomials $g_0(x) \coloneqq d$, $g_1(x) \coloneqq d \cdot x$ and $g_2(x) \coloneqq d \cdot x^2$.

We begin with $g_0(x) \coloneqq d$ and evaluate at position $x_0 \coloneqq m$:

$$\int_{-\infty}^{\infty} f_n(x) g_0(x) dx =$$

$$\int_{-\infty}^{\infty} \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2}(x-m)^2\right) \cdot d\ dx =$$

$$d \cdot \sqrt{\frac{n}{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{n}{2}(x-m)^2\right) dx =$$

$$d \cdot \sqrt{\frac{n}{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\left(\frac{n}{2}x^2 - nxm + \frac{n}{2}m^2\right)\right) dx =$$

$$d \cdot \sqrt{\frac{n}{2\pi}} \cdot \sqrt{\frac{2\pi}{n}} \cdot e^{\left(\frac{n^2m^2}{2n} - \frac{n}{2}m^2\right)} =$$

$$d \cdot \sqrt{\frac{n}{2\pi}} \cdot \sqrt{\frac{2\pi}{n}} = d$$

Result:

$$\int_{-\infty}^{\infty} f_n(x) g_0(x) dx = g_0(x_0)$$

We check the function $g_1(x) \coloneqq d \cdot x$ and evaluate at position $x_0 \coloneqq m$.

We use:

$$\int_{-\infty}^{\infty} x \cdot \exp(-a(x-b)^2) dx = b\sqrt{\frac{\pi}{a}}$$

With this we get:

$$\int_{-\infty}^{\infty} f_n(x) g_1(x) dx =$$

$$\int_{-\infty}^{\infty} \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x-m)^2\right) \cdot d \cdot x dx =$$

$$d\sqrt{\frac{n}{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{n}{2} \cdot (x-m)^2\right) \cdot x dx =$$

$$d\sqrt{\frac{n}{2\pi}} \cdot m \cdot \sqrt{\frac{2\pi}{n}} =$$

$$d \cdot m$$

Result:

$$\int_{-\infty}^{\infty} f_n(x) g_1(x) dx = g_1(x_0)$$

We try with the function $g_2(x) \coloneqq d \cdot x^2$ and evaluate at position $x_0 \coloneqq m$.

We use:

$$\int_{-\infty}^{\infty} x^2 \cdot \exp\left(-(ax^2 + bx)\right) dx = \frac{\sqrt{\pi}(2a + b^2)}{4a^{\frac{5}{2}}} \cdot e^{\frac{b^2}{4a}}$$

We have:

$$d \int_{-\infty}^{\infty} x^2 \cdot \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x - m)^2\right) dx$$

We expand:

$$d \int_{-\infty}^{\infty} x^2 \cdot \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x - m)^2\right) dx =$$

$$d\sqrt{\frac{n}{2\pi}} \cdot \int_{-\infty}^{\infty} x^2 \cdot \exp\left(-\frac{n}{2} \cdot (x - m)^2\right) dx =$$

$$d\sqrt{\frac{n}{2\pi}} \cdot \int_{-\infty}^{\infty} x^2 \cdot \exp\left(-\frac{n}{2}x^2 + nmx - \frac{n}{2}m^2\right) dx =$$

$$d\sqrt{\frac{n}{2\pi}} \cdot \int_{-\infty}^{\infty} x^2 \cdot \exp\left(-\frac{n}{2}x^2 + nmx\right) \cdot \exp\left(-\frac{n}{2}m^2\right) dx =$$

$$d\sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2}m^2\right) \cdot \int_{-\infty}^{\infty} x^2 \cdot \exp\left(-\frac{n}{2}x^2 + nmx\right) dx =$$

$$d\sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2}m^2\right) \cdot \int_{-\infty}^{\infty} x^2 \cdot \exp\left(-\left(\frac{n}{2}x^2 - nmx\right)\right) dx$$

Note: $\exp\left(-\frac{n}{2}m^2\right)$ is a constant not depending on x.

We calculate the integral:

$$\int_{-\infty}^{\infty} x^2 \cdot \exp\left(-\left(\frac{n}{2}x^2 - nmx\right)\right) dx = \frac{\sqrt{\pi}(n + n^2m^2)}{4\sqrt{\left(\frac{n}{2}\right)^5}} \cdot e^{\frac{n^2m^2}{2n}} =$$

$$\frac{\sqrt{2\pi}(n + n^2m^2)}{\sqrt{n^5}} \cdot e^{\frac{nm^2}{2}}$$

We complete calculation:

$$d\sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2}m^2\right)\frac{\sqrt{2\pi}(n+n^2m^2)}{\sqrt{n^5}} \cdot e^{\frac{nm^2}{2}} =$$

$$d \cdot \frac{(n+n^2m^2)}{n^2} =$$

$$d \cdot \left(\frac{1}{n} + m^2\right)$$

What we get is:

$$\int_{-\infty}^{\infty} d \cdot x^2 \cdot \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-\frac{n}{2} \cdot (x-m)^2\right) dx = d \cdot \left(\frac{1}{n} + m^2\right)$$

With rising n the sequence is converging to the desired result $d \cdot m^2$:

$$\int_{-\infty}^{\infty} f_n(x) g_2(x) dx = g_2(x_0)$$

We conclude: The Dirac δ-function used in the scalar product extracts a single point out of every polynomial function.

Statistics

Properties of the probability density function $p(x)$:

$$p(x) \geq 0 \; for \; all \; x$$

$$p(x) \; is \; continuous^*$$

$$\int_{-\infty}^{\infty} p(x) dx = 1$$

* Step functions allowed …

The Dirac δ-functions fulfills these properties.

If we build the probability measure from the Dirac δ-function, we get a step function:

$$P(x) := \int_{-\infty}^{x} \delta(\tau) d\tau$$

$$P(x) = \begin{cases} 0 & for \; x \leq 0 \\ 1 & for \; x > 0 \end{cases}$$

In this sense the Dirac δ-function concentrates the probability of the position of a particle to a single point.

Extended space of square integrable functions

The Dirac δ-function:

$$\delta_{x_0}(x) := \delta(x - x_0) = \begin{cases} 0 & for \; x \neq x_0 \\ \infty & for \; x = x_0 \; (*) \end{cases}$$

Note: $(*)$ maybe it is better to write "undefined" instead of ∞.

We write $\delta(x_0)$ instead of $\delta(x - x_0)$. This is a function of x with the target value x_0. The ket related is $|\delta_{x_0}\rangle$.

If we use the space of square integrable functions extended by the Dirac δ-function, we have a new basis within this space.

The set $\{|\delta_{x_0}\rangle, x_0 \in \mathbb{R}\}$ can serve as a basis of this space.

The basis vectors (functions) are orthogonal:

$$\langle\delta_{x_0}|\delta_{x_1}\rangle = \int_{-\infty}^{\infty} \delta(x_0)\delta(x_1)dx = 0\ for\ x_1 \neq x_0$$

The Dirac δ-function itself is not square-integrable:

$$\langle\delta_{x_0}|\delta_{x_0}\rangle = \int_{-\infty}^{\infty} \delta(x_0)\delta(x_0)dx\ undefined$$

Note: The Dirac δ-function is divergent, but the scalar $\langle\delta_{x_0}|\delta_{x_0}\rangle$ product rises very slowly.

The Dirac δ-functions build a complete basis:

$$f(x) = \langle\delta_{x_0}|f\rangle\ \forall x_0 \in \mathbb{R}$$

The Dirac δ-functions build a continuous basis system. A function f can be written as an integral:

$$|f\rangle = \int_{-\infty}^{\infty} |\delta_{x_0}\rangle\langle\delta_{x_0}|f\rangle\, dx = \int_{-\infty}^{\infty} f(x)|\delta_{x_0}\rangle dx$$

This is the continuous case, equivalent to the sum we use with finite dimension vectors:

$$|\vec{f}\rangle = \sum_i |\vec{e_i}\rangle\langle\vec{e_i}|\vec{f}\rangle = \sum_i f_i|\vec{e_i}\rangle$$

The Dirac δ-function is the equivalent to the unity matrix.

In the finite dimensional case:

$$id_{ij} = \langle i|id|j\rangle = \delta_{ij}$$

Note: id is the unity matrix.

In the continuous case:

$$id_{x_0x_1} = \langle\delta_{x_0}|id|\delta_{x_1}\rangle = \delta(x_0 - x_1)$$

The unit-operator becomes the integral over all projection operators $|\delta_{x_0}\rangle\langle\delta_{x_0}|$:

$$id = \int_{-\infty}^{\infty} |\delta_{x_0}\rangle\langle\delta_{x_0}|dx$$

This is the equivalent to the finite dimensional case:

$$id = \sum_i |e_i\rangle\langle e_i|$$

The vectors $|\delta_x\rangle$ are eigenvectors of the position operator X:

$Xf = \lambda f$ resp. $xf(x) = \lambda f(x)$ are fulfilled by:

$$X|\delta_{x_0}\rangle = x_0|\delta_{x_0}\rangle$$

Notation

It may be confusing that the Dirac δ-function is a function of x and targets a value x_0. We will show this with an example, one time with the notation use by Griffiths, one time with the notation of this paper. You find this example in Griffiths, 3.3 Eigenfunctions of a Hermitian Operator.

Griffiths, Example 3.3	this paper …	
Find the eigenfunctions and eigenvalues of the position operator. Solution: Let $g_y(x)$ be the eigenfunction and y the eigenvalue: $\hat{x}g_y(x) = xg_y(x) = yg_y(x)$ Here y is a fixed number (for any given eigenfunction), but x is a continuous variable. What function of x has the property that multiplying it by x is the same as multiplying it by the constant y? Obviously, it's got to be *zero*, except at the one point $x = y$; in fact, it is nothing but the Dirac δ-function: $g_y(x) = A\delta(x-y)$ This time the eigenvalue *has* to be real; the eigenfunctions are not square integrable, but again they admit *Dirac* orthonormality: $\int_{-\infty}^{\infty} g_{y'}^{*}(x) g_y(x) dx$ $= \lvert A\rvert^2 \int_{-\infty}^{\infty} \delta(x-y')\delta(x-y)dx$ $= \lvert A\rvert^2\, \delta(y-y')$ If we pick $A = 1$, so $g_y(x) = \delta(x-y)$, then $\langle g_{y'} \vert g_y \rangle = \delta(y-y')$. These eigenfunctions are also complete: $f(x) = \int_{-\infty}^{\infty} c(y)\, g_y(x) dy$ $= \int_{-\infty}^{\infty} c(y)\, \delta(x-y) dy$ with $c(y) = f(y)$	Find the eigenfunctions and eigenvalues of the position operator. Solution: Let $\delta_{x_0}(x)$ be the eigenfunction and x_0 the eigenvalue: $X\delta_{x_0}(x) = x \cdot \delta_{x_0}(x) = x_0 \cdot \delta_{x_0}(x)$ Here x_0 is a fixed number (for any given eigenfunction), but x is a continuous variable. What function of x has the property that multiplying it by x is the same as multiplying it by the constant x_0? Obviously, it's got to be *zero*, except at the one point $x = x_0$; in fact, it is nothing but the Dirac δ-function: $\delta_{x_0}(x) = A\delta(x-x_0)$ This time the eigenvalue *has* to be real; the eigenfunctions are not square integrable, but again they admit *Dirac* orthonormality: $\int_{-\infty}^{\infty} \delta_{x_1}(x)\, \delta_{x_0}(x) dx$ $= \lvert A\rvert^2 \int_{-\infty}^{\infty} \delta(x-x_1)\delta(x-x_0)dx$ $= \lvert A\rvert^2\, \delta(x_0-x_1)$ If we pick $A = 1$, so $\delta_{x_0}(x) = \delta(x-x_0)$, then $\langle \delta_{x_1} \vert \delta_{x_0} \rangle = \delta(x_0-x_1)$. These eigenfunctions are also complete: $f(x) = \int_{-\infty}^{\infty} c(x_0)\, \delta_{x_0}(x) dx_0$ $= \int_{-\infty}^{\infty} c(x_0)\, \delta(x-x_0) dx_0$ with $c(x_0) = f(x_0)$	a) b)

Note:

a) We prefer x_0 instead of y. The equation $x \cdot \delta_{x_0}(x) = x_0 \cdot \delta_{x_0}(x)$ is somewhat problematic because $\delta_{x_0}(x)$ has no existing value in the sense that there might be a real number.
b) We use the real valued Dirac δ-function, so complex conjugation doesn't change it.