

Hermiticity and its consequences

Notes on Quantum Mechanics

<http://quantum.bu.edu/notes/QuantumMechanics/HermiticityAndItsConsequences.pdf>

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In all applications of quantum mechanics in chemistry we ultimately want to understand things that we measure in the lab. The result of any measurement is always a real number. This means that we need to be sure that the procedures we develop for quantum calculations always give us correspondingly real answers.

In the Schrödinger approach to quantum mechanics, classical quantities are replaced by operators chosen to be consistent with the position-momentum commutation relation, $[x, p] = i\hbar$. There is an additional property that quantum mechanical operators satisfy, namely that they are hermitian. This requirement has several important, useful consequences described below. The most important of these is that thereby the eigenvalues are always real numbers.

■ Hermiticity

By definition, an hermitian operator q satisfies

$$\int f(x)^* q(x) g(x) dx = \int \{q(x) f(x)\}^* g(x) dx$$

To see how this definition works, let's show that the momentum operator, $p = -i\hbar d/dx$, is hermitian.

The first thing to do is to rearrange the integral as

$$\begin{aligned} & \int f(x)^* \left(-i\hbar \frac{d}{dx}\right) g(x) dx \\ &= -i\hbar \int f(x)^* \frac{d}{dx} g(x) dx \\ &= -i\hbar \int f(x)^* dg(x). \end{aligned}$$

Next, we integrate by parts,

$$\begin{aligned} &= -i\hbar \left\{ f(x)^* g(x) \Big|_{-\infty}^{\infty} - \int g(x) df(x)^* \right\} \\ &= -i\hbar \left\{ 0 - \int g(x) \frac{d}{dx} f(x)^* dx \right\}. \end{aligned}$$

The first term vanishes if we assume the functions f and g are for bound states and so that they vanish at the limits. We can then rearrange the remaining integral as

$$= \int g(x) \left(-i\hbar \frac{d}{dx} f(x)\right)^* dx$$

and so show that the momentum operator satisfies

$$\int f(x)^* \left(-i \hbar \frac{d}{dx}\right) g(x) dx = \int \left(-i \hbar \frac{d}{dx} f(x)\right)^* g(x) dx$$

which is the definition of hermiticity.

There are three important consequences of an operator being hermitian: Its eigenvalues are *real*; its eigenfunctions corresponding to different eigenvalues are *orthogonal* to one another; and the set of all its eigenfunctions is *complete*.

Examples

- | Show that the operator $+i \hbar d / dx$ is hermitian
- | Show that the operator d / dx is not hermitian
- | Use the fact that the momentum operator is hermitian to show that the kinetic energy operator is hermitian. Hint: Show that is an operator, o , is hermitian, then the operator $o^2 = o o$ is hermitian.
- | Use the fact that the operator for position is just "multiply by position" to show that the potential energy operator is hermitian. Hint: Potential energy is a function of position.
- | Use the results of the previous two questions to show that the hamiltonian, H , is hermitian.

■ Real eigenvalues

Let's use the notation that an eigenfunction relation is

$$q(x) f_j(x) = c_j f_j(x),$$

where q is an operator, f_j is its j -th eigenfunction, and the number c_j is its j -th eigenvalue. If q is hermitian, then the eigenvalues c_j are real numbers.

To see this, we begin by expressing the j -th eigenvalue in terms of the integral

$$\int f_j(x)^* q(x) f_j(x) dx = c_j$$

where in this step we assume that the eigenfunctions are normalized to 1. Next, we can use the hermiticity property to rearrange the integral on the left hand side as

$$\begin{aligned} & \int f_j(x)^* q(x) f_j(x) dx \\ &= \int (q(x) f_j(x))^* f_j(x) dx \\ &= \int (c_j f_j(x))^* f_j(x) dx \\ &= c_j^* \int f_j(x)^* f_j(x) dx \\ &= c_j^* \end{aligned}$$

But the integral is also equal to c_j and so we have that

$$c_j^* = c_j$$

This can only be true if c_j is a real number.

▮ Show that the total energy of particle in a two dimensional potential must be a real number.

■ Orthogonal functions

If f_j and f_k are eigenfunctions of the same hermitian operator but correspond to different eigenvalues, $c_j \neq c_k$, then they are orthogonal to one another, in the sense that

$$\int f_j(x)^* f_k(x) dx = 0.$$

To see this, we begin with the integral relation

$$\int f_j(x)^* q(x) f_k(x) dx = c_k \int f_j(x)^* f_k(x) dx.$$

Next, we can use the hermiticity property to rearrange the integral on the left hand side as

$$\begin{aligned} \int f_j(x)^* q(x) f_k(x) dx &= \int (q(x) f_j(x))^* f_k(x) dx \\ &= \int (c_j f_j(x))^* f_k(x) dx \\ &= c_j \int f_j(x)^* f_k(x) dx, \end{aligned}$$

where in the last line we use the fact that the eigenvalues are real. Subtracting these two alternative expressions for the integral, we get

$$0 = (c_j - c_k) \int f_j(x)^* f_k(x) dx.$$

If the eigenvalues are different, then $c_j - c_k \neq 0$, and so the only way the equation can be true is if the integral vanishes,

$$\int f_j(x)^* f_k(x) dx = 0.$$

that is, the eigenfunctions corresponding to different eigenvalues are orthogonal.

We can express the orthogonality of different eigenfunctions and the normalization of each eigenfunction in a single *orthonormality relation*,

$$\int f_j(x)^* f_k(x) dx = \delta_{jk},$$

in terms of the *Kronecker delta* symbol δ_{jk} . The value of δ_{jk} is 0 if $j \neq k$ and is 1 of $j = k$.

What is the value of $\sum_{j=1}^5 \delta_{j6}$?

What is the value of $\sum_{j=1}^{11} \delta_{j6}$?

What is the value of $\sum_{j=1}^{11} \delta_{j6} f_j$?

Examples

The normalized wavefunctions for a particle in an infinite well of width L are

$$\psi_j(x) = \sqrt{2/L} \sin(j\pi x/L).$$

Make a plot of the product $\psi_2(x)\psi_3(x)$ for $L = 1$ and use it to assess whether the sum, $\int_0^1 \psi_2(x)^* \psi_3(x) dx$, is zero.

Which of the following integrals must be zero? Hint: The infinite well hamiltonian is hermitian.

$$\int_0^1 \psi_2(x)^* \psi_2(x) dx,$$

$$\int_0^1 \psi_2(x)^* \psi_3(x) dx,$$

$$\int_0^1 \psi_2(x)^* \psi_4(x) dx,$$

$$\int_0^1 \psi_1(x)^* \psi_5(x) dx.$$

Here are the hydrogen atom 1s, 3s, 3d, and 5d radial wavefunctions.

$$\begin{array}{ll} 1s & 2 e^{-r} r \\ 3s & \frac{2 e^{-r/3} r (27-18r+2r^2)}{81\sqrt{3}} \\ 3d & \frac{2}{81} \sqrt{\frac{2}{15}} e^{-r/3} r^3 \\ 5d & \frac{2\sqrt{\frac{2}{35}} e^{-r/5} r^3 (525-70r+2r^2)}{46875} \end{array}$$

Make a plot of the product $f_{1s}(r) f_{3s}(r)$ and use it to assess whether the sum, $\int_0^\infty f_{1s}(r)^* f_{3s}(r) dr$, is zero.

Which of the following integrals must be zero? Hint: The one-electron-atom hamiltonian for radial motion is hermitian.

$$\int_0^\infty f_{1s}(r)^* f_{3s}(r) dr,$$

$$\int_0^\infty f_{1s}(r)^* f_{3d}(r) dr,$$

$$\int_0^\infty f_{3s}(r)^* f_{3d}(r) dr,$$

$$\int_0^\infty f_{3d}(r)^* f_{5d}(r) dr.$$

■ Completeness prelude: Dirac delta function

The third property of solutions ψ_j to a Schrödinger equation is that they form a *complete set*. The term complete is used in the sense that the any function, Ψ , satisfying the same general conditions may be expressed as a linear combination of the functions that form the complete set,

$$\Psi(x) = \sum_j \psi_j(x) c_j = \psi_1(x) c_1 + \psi_2(x) c_2 + \psi_3(x) c_3 + \dots,$$

where the sum is over all of the members of the complete set.

In order to use completeness in mathematical manipulations, Dirac, one of the developers of quantum mechanics, found it necessary to introduce a new kind of mathematical function, known as the *delta function*, $\delta(x' - x)$. Dirac defined the function to have the following peculiar properties. The delta function is

- is zero everywhere except when its argument is zero, that is except when $x' = x$,
- at $x = x'$ it is ∞ ,
- but its total area, including the infinitely high peak, is equal to one!

Because the delta function is infinite when its argument is zero, it is zero elsewhere, but it integrates to 1, it is not a function in the usual sense. The problem is that its numerical value does not vary smoothly from $x' - x \neq 0$ (where it is 0) to $x' - x = 0$, (where it is infinite). For this reason, the delta function is always used only as a factor in an integrand, and its effect there is to select out that part of the other factors in the integrand for which $x' = x$.

A good way to see all of these aspects together is to consider the integral of the product of a "normal" function, $f(x')$, and the delta function. The product has the value 0 everywhere except where $x' = x$ (that is, where the function f has the value $f(x)$). The key point is that integrating the product over all values of x gives just $f(x)$,

$$\int f(x') \delta(x' - x) dx' = f(x).$$

|| Show that a special case of this result is that

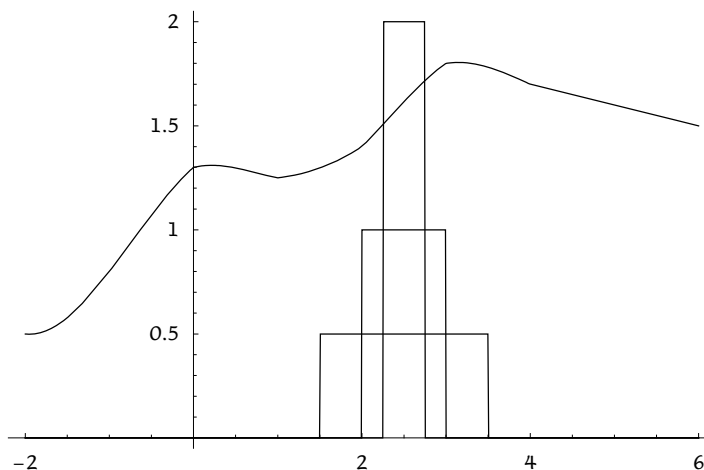
$$\int_{-\infty}^{\infty} \delta(x' - x) dx' = 1.$$

|| Evaluate the following integral.

$$\int_{-\infty}^{\infty} e^{x'^2} \sin(4\pi x') \delta(x' - x) dx'.$$

|| The answer to this problem may convince you that working with the delta function is quite easy.

A way to think about the delta function is that it acts a filter through which only the value of f at $x' = x$ is able to pass. We can illustrate this *filtering property* of a Dirac delta function by graphing an approximation to it. (We cannot graph the delta function itself, since its single non-zero value is infinite.) Here are three "rectangle" functions $g_{\text{rect}}(x - x')$, each of area 1 and centered at $x' = 2.5$ but successively narrower widths w .



Rectangle functions g_{rect} of area 1 and function $f(x)$. The average value of $f(x)$ for the successively smaller rectangles is 1.602, 1.610, and 1.614. In the limit of zero width, the average value is $f(2.5) = 1.615$.

Now, consider the integral

$$\int_{-\infty}^{\infty} f(x) g_{\text{rect}}(x - 2.5) dx.$$

The integrand vanishes except where g_{rect} is not zero, and so is equal to

$$\int_{x'-w/2}^{x'+w/2} f(x) g_{\text{rect}}(x - 2.5) dx.$$

If w is small enough so that $f(x)$ does not change much in the region $x - w/2 \leq x \leq x + w/2$, then the integral is approximately equal to

$$\int_{x'-w/2}^{x'+w/2} f(x) g_{\text{rect}}(x - 2.5) dx \approx \langle f(x) \rangle_w \int_{x'-w/2}^{x'+w/2} g_{\text{rect}}(x - 2.5) dx$$

where $\langle f(x) \rangle_w$ is the average value of $f(x)$ in the region,

$$\langle f(x) \rangle_w = \frac{1}{w} \int_{x'-w/2}^{x'+w/2} f(x) dx.$$

The average value of $f(x)$ for the successively smaller rectangles shown in the figure is 1.602, 1.610, and 1.614. In the limit of zero width, the average value is $\langle f(x) \rangle_{w \rightarrow 0} = f(2.5) = 1.615$. As w shrinks toward zero, $\langle f(x) \rangle$ is closer and closer to the value of f at the center of the region, $f(2.5)$. In the limit $w \rightarrow 0$, $g(2.5) \rightarrow \infty$ while the area under g_{rect} remains 1, and so

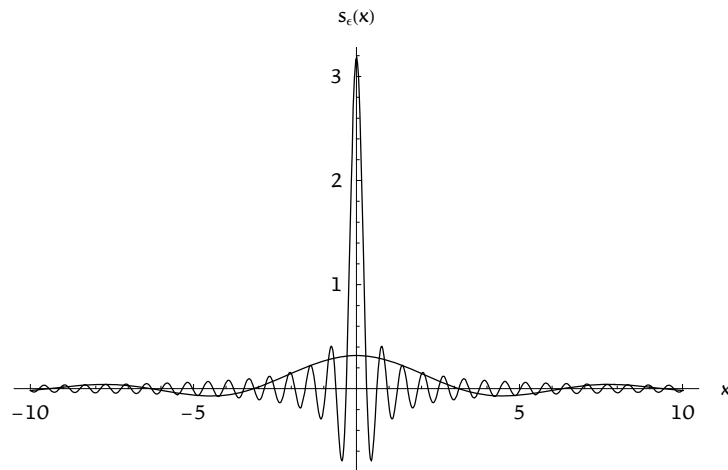
$$\lim_{w \rightarrow 0} \int_{x'-w/2}^{x'+w/2} f(x) g_{\text{rect}}(x - 2.5) dx \approx f(2.5) = 1.615.$$

In this way we see can understand first, what is meant by the Delta function being a function that is zero everywhere except $x = x'$ where it is infinite height and that has unit area unit area, and second, that such a function used as a factor in an integrand act as a filter to select out the value of the rest of the integrand at $x = x'$.

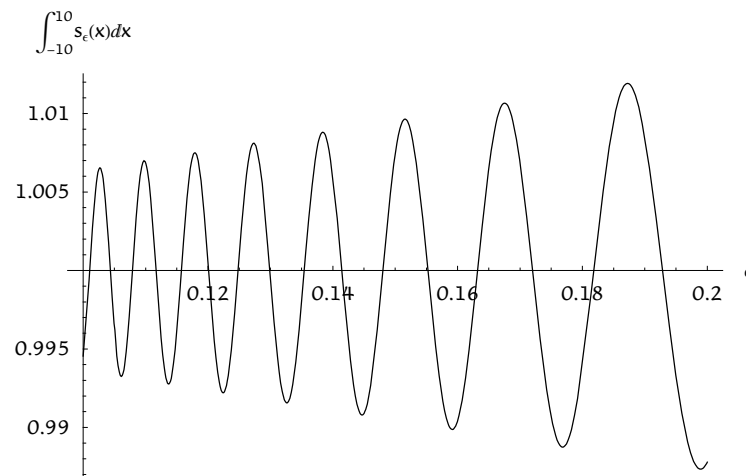
Rectangle functions are one of many examples of approximations to a delta function. Another example of an approximation to the delta function is

$$s_\epsilon(x) = \frac{1}{\pi} \frac{\sin(x/\epsilon)}{x},$$

which behaves more and more as a delta function the smaller the value of ϵ . To see this, here is a plot of this function for $\epsilon = 1$ (low, broad peak) and $\epsilon = 0.1$ (narrow, high peak).



The key feature of the function $s_\epsilon(x)$ is that its integral is close to one, the more so the smaller the value of ϵ . This behavior is illustrated in the following plot of the value of the integral $\int_{-10}^{10} s_\epsilon(x) dx$ for values of ϵ from 0.1 to 0.2.



From this behavior we extrapolate that in the limit $\epsilon \rightarrow 0$, $s_\epsilon(x)$ is zero everywhere except at $x = 0$, where it is infinite, and that its integral over all space is one. That is, we conclude that

$$\lim_{\epsilon \rightarrow 0} s_\epsilon(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \frac{\sin(x/\epsilon)}{x} = \delta(x).$$

There are many other approximations to the delta function. They share the feature that they become exact only in a limit. We'll learn about a particular class of these approximations when we discuss some of the formal aspects of quantum theory. We'll also see how the delta function makes it possible for use to normalize unbound wave functions, even though they oscillate about zero out to infinite distance.

■ Completeness

A way to understand the idea of completeness is to consider the analogous problem of expressing a vector in terms of its components. (These components are the vector analogues of the coefficients c_j .) In three dimensions we can express an arbitrary vector, \vec{r} , as

$$\vec{r} = \hat{i} r_x + \hat{j} r_y + \hat{k} r_z,$$

in terms of the components, $r_x = \hat{i} \cdot \vec{r}$, etc., along the three orthogonal axes and the unit vectors along those axes. Now, we can rearrange this expansion as follows:

$$\vec{r} = \hat{i} r_x + \hat{j} r_y + \hat{k} r_z = \hat{i} \hat{i} \cdot \vec{r} + \hat{j} \hat{j} \cdot \vec{r} + \hat{k} \hat{k} \cdot \vec{r} = (\hat{i} \hat{i} + \hat{j} \hat{j} + \hat{k} \hat{k}) \cdot \vec{r}.$$

Comparing the first and last expressions, it is evidently so that

$$1 = \hat{i} \hat{i} + \hat{j} \hat{j} + \hat{k} \hat{k}$$

in the sense of an operator identity. This identity is known as the *completeness relation* for the unit vectors of the three dimensional space. The quantities $\hat{i} \hat{i}$, etc., are known as dyadics, and the implied operation is the dot product. Dyadics are special in that they behave like two samurai warriors standing back to back, at the ready to fend off as a pair attackers that may come from any direction,

$$\vec{r} \cdot \hat{i} \hat{i} = r_x \hat{i},$$

$$\hat{i} \hat{i} \cdot \vec{r} = \hat{i} r_x.$$

The unit vector completeness relation is a compact statement of the fact that any vector in three dimensional space may be expressed in terms of its components along the units vectors of the space.

Express the vector of length 4.21 directed along $\theta = 45.3^\circ$, $\phi = 113^\circ$ in terms of the unit vectors \hat{i} , \hat{j} and \hat{k} . Answer: $\vec{r} = -\hat{i} 2.75 + \hat{j} 1.17 + \hat{k} 2.96$.

{-1.16925, 2.75458, 2.96129}

The generalization of the unit vector completeness relation to a set of functions is

$$\delta(x' - x) = \sum_j \psi_j(x) \psi_j^*(x'),$$

where the sum is over all of the eigenfunctions of the complete set.

Because delta functions take on infinite values, but integrate to 1, they are not functions in the usual sense; that is, their numerical value does not vary smoothly from $x \neq x'$ to $x = x'$. For this reason, Dirac delta functions are always used only as elements of an integrand, and their effect there, as we have seen, is to select out that part of the integrand for which $x' = x$,

$$\int f(x') \delta(x' - x) dx' = f(x).$$

Earlier we illustrated the *filtering property* of a Dirac delta function by graphing successively better approximations to it.

We can explore delta functions expressed as sums of products of eigenfunctions in the same way. To do this, however, we need to take account of a practical complication: Since typically the number of

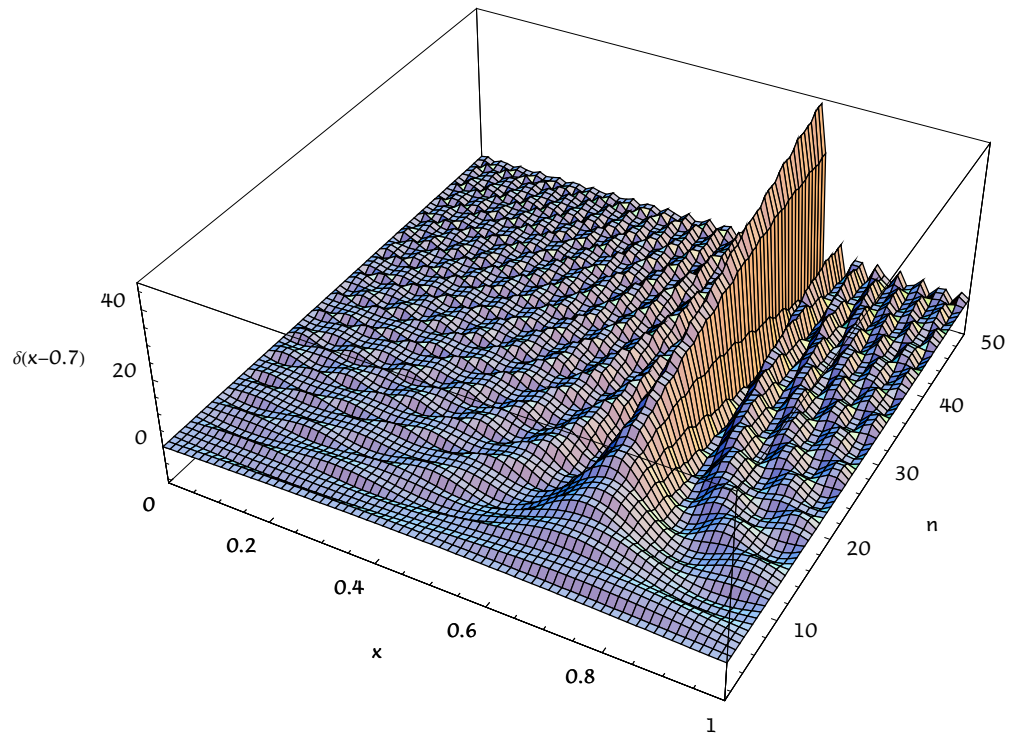
eigenfunctions of an operator is infinite, the definition of the Dirac delta function has an infinite number of terms. Since we can only work with a finite number of terms in any numerical evaluation of the sum, the best we can do is to approximate the sum in terms of a finite number, n , of products of functions from a particular basis,

$$\delta(x' - x) \approx \sum_{j=1}^n \psi_j^*(x') \psi_j(x).$$

The more terms we include in the sum, the better the approximation.

Square-well approximation to the delta function

Here are successively better approximations to a Dirac delta function centered at $x = 0.7$, using a square-well basis for a well extending from $x = 0$ to $x = 1$.

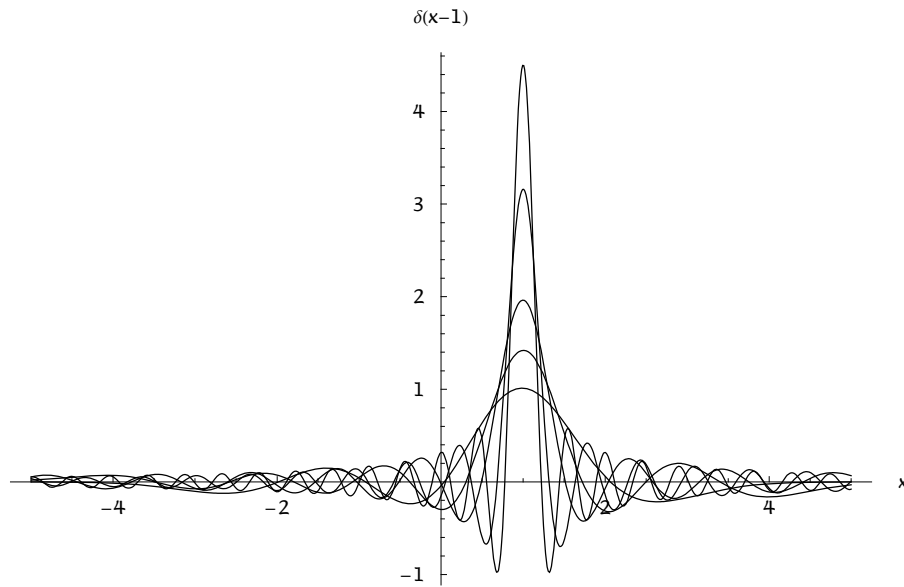


Approximations to Dirac delta function $\delta(x - 0.7)$ using a finite (and so incomplete) square well basis. The approximations correspond to the including the first n square well functions, from just one to 50 basis functions, in the Dirac delta function sum. The central peak becomes narrower and higher as more basis functions are included. In the limit of an infinite number of basis functions, the central peak would have zero width, infinite height, and area 1.

The more terms included in the sum, the better the approximation. The approximation becomes exact in the limit of including the infinite number of square-well wavefunctions in the sum.

Harmonic oscillator approximation to the delta function

Here are successively better approximations to a Dirac delta function centered at $x = 1$, using a harmonic oscillator basis.



Approximations to Dirac delta function $\delta(x-1)$ using a finite (and so incomplete) harmonic oscillator basis. The five approximations correspond to the including the first 5 (lowest central peak), 10, 20, 50, and 100 (highest central peak) harmonic oscillator basis functions in the Dirac delta function sum. The central peak becomes narrower and higher as more basis functions are included. In the limit of an infinite number of basis functions, the central peak would have zero width, infinite height, and area 1.

The more terms included in the sum, the better the approximation. The approximation becomes exact in the limit of including the infinite number of harmonic oscillator wavefunctions in the sum.

■ Comparison of vector and function completeness relations

Once we have extended the idea of completeness to functions, we can proceed by analogy with basis vectors in three dimensional space to express a function, $\Psi(x)$, in terms of a basis of functions, $\psi_j(x)$.

Completeness relation:

$$1 = \hat{i}\hat{i} + \hat{j}\hat{j} + \hat{k}\hat{k}, \text{ unit vectors in three dimensional space}$$

$$\delta(x' - x) = \sum_j \psi_j^*(x') \psi_j(x), \text{ basis functions in infinite dimensional (Hilbert) space}$$

Orthonormality:

$$\hat{i} \cdot \hat{j} = \delta_{ij}$$

$$\int \psi_i(x)^* \psi_j(x) dx = \delta_{ij}$$

Expansion in basis:

$$\begin{aligned} \vec{r} &= (\hat{i}\hat{i} + \hat{j}\hat{j} + \hat{k}\hat{k}) \cdot \vec{r} \\ &= \hat{i}r_x + \hat{j}r_y + \hat{k}r_z, \text{ vector expanded in basis of unit vectors} \end{aligned}$$

$$\begin{aligned}
\Psi(x) &= \int \Psi(x') \sum_j \psi_j^*(x') \psi_j(x) dx' \\
&= \sum_j \psi_j(x) \int \Psi(x') \psi_j^*(x') dx' \\
&= \sum_j \psi_j(x) c_j \\
&= \psi_1(x) c_1 + \psi_2(x) c_2 + \psi_3(x) c_3 + \dots, \text{ function expanded in basis of functions}
\end{aligned}$$

Expansion coefficients:

$$r_x = \hat{i} \cdot \vec{r}, \text{ etc., projection of vector along unit vector}$$

$$c_1 = \int \psi_1(x)^* \Psi(x) dx, \text{ etc., "projection" of function "along" basis function}$$

There are two ways this expansion scheme is used. First, by expressing a known function in terms of basis functions, expectation values can be expressed in terms of those of the basis functions.

Assume an electron in a square well is prepared in the superposition of square well states $\Psi = \sqrt{0.2} \psi_1 + \sqrt{0.5} \psi_2 + \sqrt{0.3} \psi_3$. Show that $\sqrt{0.2} = \int \psi_1(x)^* \Psi(x) dx$.

Show that Ψ is normalized to 1. Hint: Evaluate $\int \Psi(x)^* \Psi(x) dx$.

Derive an expression for the energy of the electron described by Ψ . Hint: Evaluate the expectation value of the square well hamiltonian, $\langle H \rangle = \int \Psi(x)^* H \Psi(x) dx$. Answer: $0.6125 h^2 / (m L^2)$.

Second, by expressing an unknown function in terms of basis functions, the expansion coefficients can be treated as unknown parameters, and then the Schrödinger equation used to generate a linear system whose solution is the values of the expansion coefficients. This latter technique is used in most numerical solutions of the Schrödinger equation for many-electron atoms and molecules. We will discuss it further when we take up various methods of approximations used in quantum chemical calculations.

■ Effect of interactions on wavefunctions

Since the Hamiltonian is hermitian, its eigenfunctions form a complete set. We can use this completeness to analyze the effect of an interaction on a system that is in an energy eigenstate. In this way, for example, we can understand how the interaction of an oscillating electric field (light) mixes different states. Because of the universality of completeness, the analysis we now is the basis of the general framework for treating interactions in quantum system.

Let represent the interaction by the operator op . The effect of op is to alter any eigenstate of the system. Formally, this means that

$$op \psi_i(x) = f_i(x) \neq \text{constant} \times \psi_i(x).$$

that is, $f_i(x)$ is generally different from $\psi_i(x)$. Whatever $f_i(x)$ is, we can always use the completeness of the energy eigenstates to see that $f_i(x)$ is a mixture of energy eigenstates.

$$f_i(x) = \int f_i(x') \delta(x' - x) dx' = \int f_i(x') \sum_j \psi_j^*(x') \psi_j(x) dx' = \sum_j \psi_j(x) c_{j,i},$$

where

$$c_{j,i} = \int \psi_j^*(x') f_i(x') dx' = \int \psi_j^*(x') \text{op} \psi_i(x') dx'.$$

Because $c_{j,i}$ is characterized by two indices, it is called the j, i -th *matrix element* of the operator op .

Now, we can treat $f_i(x)$ as a probability amplitude and then use the Born recipe to calculate the corresponding probability density,

$$|f_i(x)|^2 = \left(\sum_k \psi_k(x) c_k \right)^* \sum_j \psi_j(x) c_j.$$

The total probability is

$$\begin{aligned} \int |f_i(x)|^2 dx &= \\ \int \left(\sum_k \psi_k(x) c_k \right)^* \sum_j \psi_j(x) c_j dx &= \sum_j |c_{j,i}|^2 \int |\psi_j(x)|^2 dx = \sum_j |c_{j,i}|^2, \end{aligned}$$

where in the second to last equality we use the fact that the eigenfunctions for different energies are orthogonal, and in the last equality we assume that the eigenfunctions are normalized. This means that

$$|c_{j,i}|^2 = \left| \int \psi_j^*(x') \text{op} \psi_i(x') dx' \right|^2$$

is the relative probability that the effect of the interaction (represented by the operator op) is to change the system from state ψ_i to state ψ_j . This is a general result: The probability of a transition is always proportional to the squared modulus of the corresponding matrix element.

Here is an example. The effect of the oscillating electric field of light polarized along the x axis is to create an oscillating electric dipole, proportional to its displacement x along the electric field direction. This means that the operator for the interaction with light is proportional to x , and so the probability of a transition from state ψ_i to state ψ_j is proportional to

$$|c_{j,i}|^2 = \left| \int \psi_j^*(x') x' \psi_i(x') dx' \right|^2$$

For a particle confined to the region $0 \leq x \leq 1$, the wavefunctions are

$$\text{psi}[j_, x_] := \sqrt{2} \sin[j \pi x]$$

and the squared matrix elements for the first ten energy levels are

```
vals = Integrate[psi[#, x] (x - 1/2) psi[1, x], {x, 0, 1}]^2 & /@ Range[10] // N
{0., 0.0324456, 0., 0.000207652, 0.,
 0.000015762, 0., 2.66931 × 10-6, 0., 6.83974 × 10-7}
```

Here the interaction operator is $\text{op} = x - 1/2$, since the induced dipole is with respect to the center of the region. The total of the squared matrix elements is

```
valsTotal = Plus @@ vals
```

```
0.0326723
```

and so the normalized probabilities are

```
vals / valsTotal
```

```
{0., 0.993059, 0., 0.00635558, 0.,  
0.000482426, 0., 0.0000816992, 0., 0.0000209343}
```

Here is how to interpret these numbers. Since the initial state has an odd number of loops (one loop), all of the transitions to states with odd numbers of loops ($1 \rightarrow 3$, $1 \rightarrow 5$, etc.) have zero probability, since by symmetry their matrix elements vanish; we say such transitions are *forbidden*. All of the transitions to states with even numbers of loops ($1 \rightarrow 2$, $1 \rightarrow 4$, etc.) have non zero probability; we say such transitions are *allowed*. The most probable allowed transition is $1 \rightarrow 2$, with relative probability 0.993. The next most probable transition is $1 \rightarrow 4$, with probability 0.006. The total probability for all of the remaining allowed transitions is $1 - (0.993 + 0.006) = 0.001$.

Repeat this analysis for transitions from the state $\psi_2 = \sqrt{2} \sin(2\pi x)$, to show that the normalized probabilities to the lowest ten energy levels are the following.

```
{0.459, 0., 0.536, 0., 0.00478, 0., 0.000444, 0., 0.0000857, 0.}
```

Construct the spectrum that represents the effect of light on a particle confined to the region $0 \leq x \leq 1$ and initially in the second energy level. Do this by drawing vertical lines of heights proportional to the corresponding transition probability and spacing corresponding to the transition energy. Express energy in units such that the energy of the lowest energy level is $E_1 = 1$.