Notes for Quantum Mechanics

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Updated for 2005

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{2005, 10, 7, 20, 58, 50.2551168}
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Lecture 4
Expansion of functions - e.g. Fourier Series as an example

Fourier Series and the Orthogonality of sines and cosines

The expansion of a function via a set of basis functions is an important one in quantum mechanics. Here is a review.

The set of functions $\{\sqrt{\frac{2}{L}} \cos \frac{2\,m\pi x}{L}, \sqrt{\frac{2}{L}}\ \sin \frac{2\,n\pi x}{L}\}$ form a complete set of orthogonal functions over the interval -L/2 to L/2. (we will take L=1 so the interval will be -.5 to .5)

What is orthogonality?

A set of functions $\{\phi_k(x)\}$ is orthogonal on a≤x≤b if for any two functions in the set $\phi_m(x)$ and $\phi_n(x)$, the following condition holds

$\int_a^b \phi_m(x)\, \phi_n(x)\, dx = \left\{ \begin{matrix} 0 \text{ if } m \neq n \\ r \text{ if } m = n \end{matrix} \right\} = r\delta_{mn}$ As you might guess we will always normalize the ϕ's so that r=1 (1)

As a reminder $\delta_{mn} = \left\{ \begin{matrix} 0 \text{ if } m \neq n \\ 1 \text{ if } m = n \end{matrix} \right.$ This thing is called the Kronecker delta (2)

A set of orthonormal things (a more general term than functions since I really want to say orthonormal kets) which span the space is a good set of base things and we can write anything in that space as a linear combination of those things.

That is $f(x) = \sum_{i=0}^{\infty} c_i\, \phi_i(x)$. I will show you later how to find the c_i's (3)

A few things to make this more clear.

First lets think of three things which we all know which form the base things for 3-space- the three unit vectors $\hat{x}$, $\hat{y}$, $\hat{z}$. These are an example of 3 base "kets" if you will let me use the term. But these are not functions - you say. OK, they are things which exist is a space - in this case 3-D space. Things can exist in other spaces - function space for instance (as in the case of the sines and cosines). I will talk next time about "juice" space. This is a space I made up which consists of juice in your refrigerator. OK, now lets check to see the three unit vectors are orthogonal. First let me denote them in a slightly different notation as $\hat{x}_1 = \hat{x}$, $\hat{x}_2 = \hat{y}$, $\hat{x}_3 = \hat{z}$. Now the thing that may be a bit confusing is that instead of the operation of integrating over a region, the relevant operation will be the dot product. Later we will use the more general notation of bra's and ket's which will take care of this. We know for example that $|\hat{x}_1|^2 = 1$ and $\hat{x}_1 \cdot \hat{x}_2 = 0$. We can write this as $\hat{x}_m \cdot \hat{x}_n = \left\{ \begin{matrix} 0 \text{ if } m \neq n \\ 1 \text{ if } m = n \end{matrix} \right\} = \delta_{mn}$ and we can see that this is the orthogonality condition..

And we also know that ANY vector $\hat{a} = \sum_{i=1}^{3} c_i \hat{x}_i$

Now you may be confused with the sines and cosines. What in the thing that plays the role of 3-D space? Its something called a functions space. As you might note, it has not just 3, but an infinite number of dimensions since m and n go from 0 to ∞. Its going to get even stranger, because you might be able to argue that function space is just an artifact of how we think about a set of functions. That might be right, but we are going to find that QM will force us into thinking about spaces which have no easy way to think about them. They are genuine new spaces which we enter when we start QM. Its as if you enter a new dimension... Welcome to the twilight zone.

OK lets get back to sines and cosines. First lets check and see if the set of functions $\{\cos \frac{2 m\pi x}{L}, \sin \frac{2 n\pi x}{L}\}$ are orthogonal.

First to make life easy, lets normalize them.

$\int_{-\frac{L}{2}}^{\frac{L}{2}} \sin \frac{2 n\pi x}{L} \sin \frac{2 n\pi x}{L} dx = \frac{L}{2}$ and $\int_{-\frac{L}{2}}^{\frac{L}{2}} \cos \frac{2 n\pi x}{L} \cos \frac{2 n\pi x}{L} dx = \frac{L}{2}$: Look this up in a integral table or just remember that the average of a function squared over its range is $\frac{1}{2}$ i.e. $\frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin \frac{2 n\pi x}{L} \sin \frac{2 n\pi x}{L} dx = \frac{1}{2}$ etc.

so our set of functions will be $\{\sqrt{\frac{2}{L}} \cos \frac{2 m\pi x}{L}, \sqrt{\frac{2}{L}} \sin \frac{2 n\pi x}{L}\}$

So now we should check that

$\frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin \frac{2 m\pi x}{L} \cos \frac{2 n\pi x}{L} dx = \text{for all } m \text{ and } n$

$\frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin \frac{2 m\pi x}{L} \sin \frac{2 n\pi x}{L} dx = \delta_{mn}$

$\frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos \frac{2 m\pi x}{L} \cos \frac{2 n\pi x}{L} dx = \delta_{mn}$

OK, now lets actually do the integrals and see. To make life easy, we will set L=1. We will do this in class. Here is one example. If you have mathematica just change m, n, and the Sin and Cos as you wish. The plots show the first function, the second function, the product of the two, and the final plot just shows the value of the integral on the y axis.

m=1

n=2

```
1
```

```
2
```

f[x_]:=Sin[2*m*Pi*x]


```
g[x_]:=Sin[2*n*Pi*x]
```

```
a=Integrate[2 * f[x] * g[x],{x,-.5,.5}]
```

7.79432×10^{-49}

```
Show[GraphicsArray[{
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{{Thickness[0.01],RGBColor[0,0,1]}}]
   },{
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    ]
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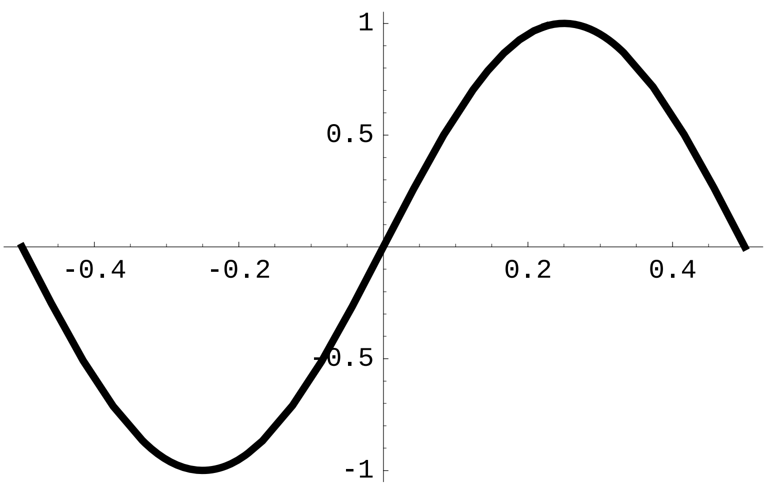

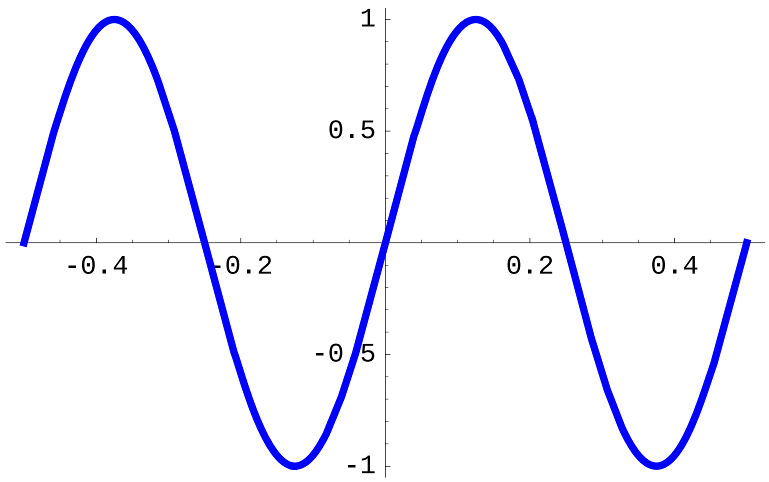
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-1
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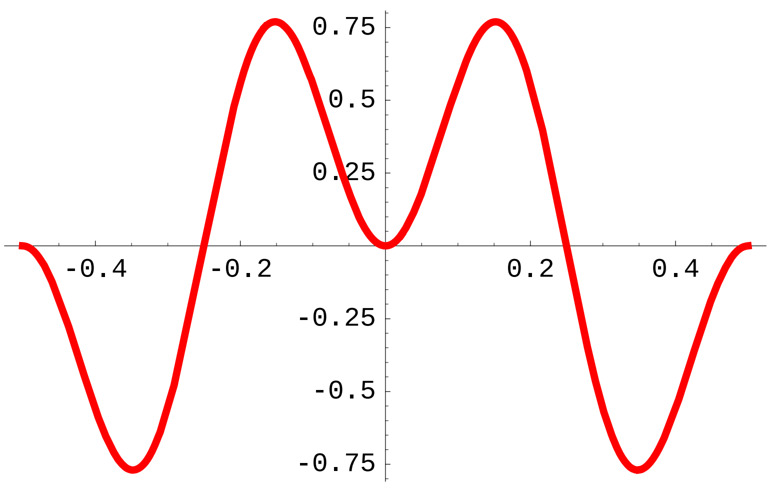
0.2
0.4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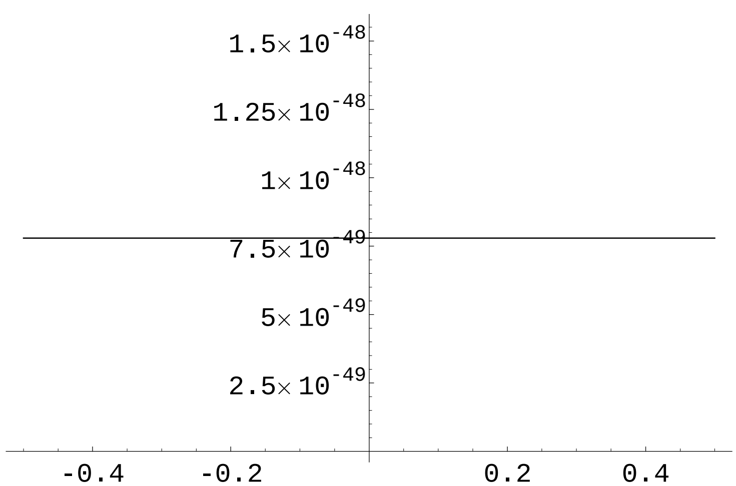
0.25
-0.25
-0.5
-0.75
-0.4
-0.2
0.2
0.4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1.25×10^{-48}
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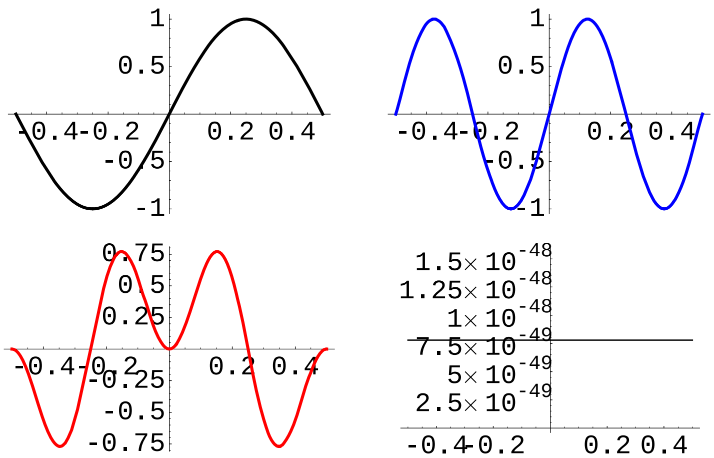
0.2
0.4



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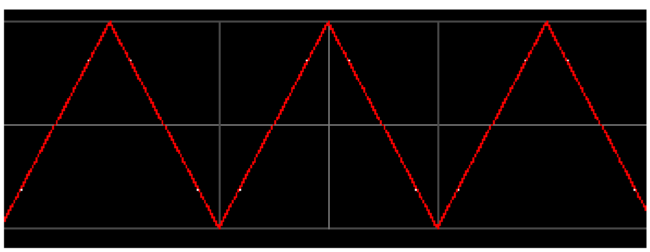
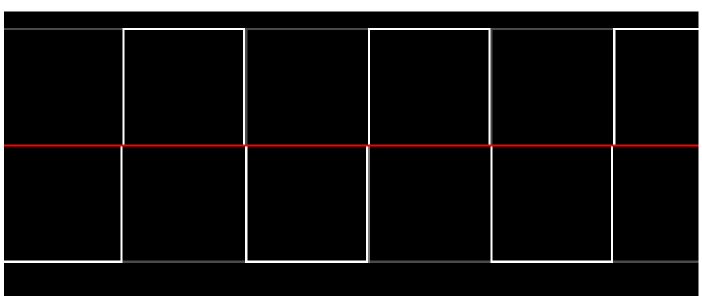
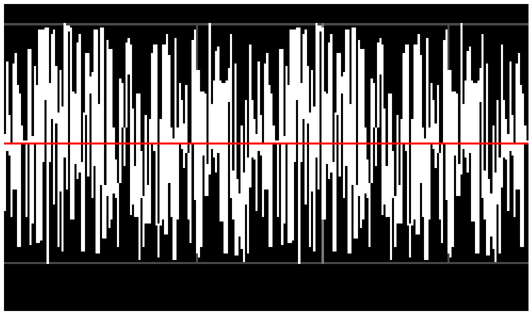
■ Fourier Series

OK now lets talk about Fourier series - which is THIS particular incarnation of the expansion into eigenkets. Other expansions you will use as far as functions will be the spherical harmonics which live in a function space similar to sines and cosines. Of course then we will get to spin which live in a completely different and alien space.

First we have to set up the rules. We are going to look at a function f(x) defined over an interval $\frac{-L}{2}$ to $\frac{L}{2}$. Later we will go from -∞ to ∞. So since it is only defined over the interval $\frac{-L}{2}$ to $\frac{L}{2}$ we will assume that the functions are periodic, *i.e.* $f(x+L) = f(x)$. Its doesn't matter. For instance it can be a sawtooth function, a square, or even white noise.







So now we can expand f(x) as a function of these sine's and cosine's $f(x)=\sum_{n=0}^{\infty}\left[a_n \sqrt{\frac{2}{L}} \cos \frac{2 n\pi x}{L} + b_n \sqrt{\frac{2}{L}} \sin \frac{2 n\pi x}{L}\right]$

Now lets solve for the a_n's and b_n's as follows. First multiplity both sides by $\sqrt{\frac{2}{L}} \cos \frac{2 m\pi x}{L}$ and integrate

$$\sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos \frac{2 m\pi x}{L}\, dx = \sum_{n=0}^{\infty}\left[a_n \int_{-\frac{L}{2}}^{\frac{L}{2}} \sqrt{\frac{2}{L}} \cos \frac{2 m\pi x}{L} \sqrt{\frac{2}{L}} \cos \frac{2 n\pi x}{L}\, dx + b_n \int_{-\frac{L}{2}}^{\frac{L}{2}} \sqrt{\frac{2}{L}} \cos \frac{2 m\pi x}{L} \sqrt{\frac{2}{L}} \sin \frac{2 n\pi x}{L}\, dx\right]$$

note that $\int_{-\frac{L}{2}}^{\frac{L}{2}} \sqrt{\frac{2}{L}} \cos \frac{2 m\pi x}{L} \sqrt{\frac{2}{L}} \cos \frac{2 n\pi x}{L}\, dx = \delta_{mn}$ So we have

$$\sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos \frac{2 m\pi x}{L}\, dx = \sum_{n=0}^{\infty}\left[a_n \delta_{mn} + b_n 0\right] = a_m$$

simillaly for b_m

So we will have

$a_n = \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos \frac{2 n\pi x}{L}\, dx$ and $b_n = \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \sin \frac{2 n\pi x}{L}\, dx$

Now lets try this for some function- Let's try the square wave so

$$f(x)=\begin{cases} -1 \text{ for } -\frac{L}{2} < x < 0 \\ 1 \text{ for } 0 < x < \frac{L}{2} \end{cases}$$

we get now

$$a_n = \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{0} (-1) \cos \frac{2 n\pi x}{L}\, dx + \sqrt{\frac{2}{L}} \int_{0}^{\frac{L}{2}} (1) \cos \frac{2 n\pi x}{L}\, dx = -\sqrt{\frac{2}{L}} \frac{L}{2 n\pi} \sin \frac{2 n\pi x}{L}\Big|_{\frac{-L}{2}}^{0} + \sqrt{\frac{2}{L}} \frac{L}{2 n\pi} \sin \frac{2 n\pi x}{L}\Big|_{0}^{\frac{L}{2}}$$
$$= \sqrt{\frac{L}{2 n^2 \pi^2}}\,[-(0-0)+0-0] = 0$$

$$b_n = \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{0} (-1) \sin \frac{2 n\pi x}{L}\, dx + \sqrt{\frac{2}{L}} \int_{0}^{\frac{L}{2}} (1) \sin \frac{2 n\pi x}{L}\, dx = \sqrt{\frac{2}{L}} \frac{L}{2 n\pi} \cos \frac{2 n\pi x}{L}\Big|_{\frac{-L}{2}}^{0} -$$
$$\sqrt{\frac{2}{L}} \frac{L}{2 n\pi} \cos \frac{2 n\pi x}{L}\Big|_{0}^{\frac{L}{2}} = \begin{cases} \sqrt{\frac{L}{2 n^2 \pi^2}}\,[1-(-1)-(-1-1)] = \sqrt{\frac{8 L}{n^2 \pi^2}} & \text{for } n \text{ odd and} \\ \sqrt{\frac{L}{2 n^2 \pi^2}}\,[1-(+1)-(+1-1)] = 0 & \text{for } n \text{ even} \end{cases}$$

So

$$f(x) = \sum_{n=\text{odd}}^{\infty} \sqrt{\frac{8 L}{n^2 \pi^2}} \sqrt{\frac{2}{L}} \sin \frac{2 n\pi x}{L} = \sum_{n=\text{odd}}^{\infty} \frac{4}{n\pi} \sin \frac{2 n\pi x}{L}$$

$$f[\text{x\_}, \text{n\_}] := \frac{4}{n*\text{Pi}}\,\text{Sin}[2*n*\text{Pi}*x]$$

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Plot[f[x, 1], {x, -1., 1.}]
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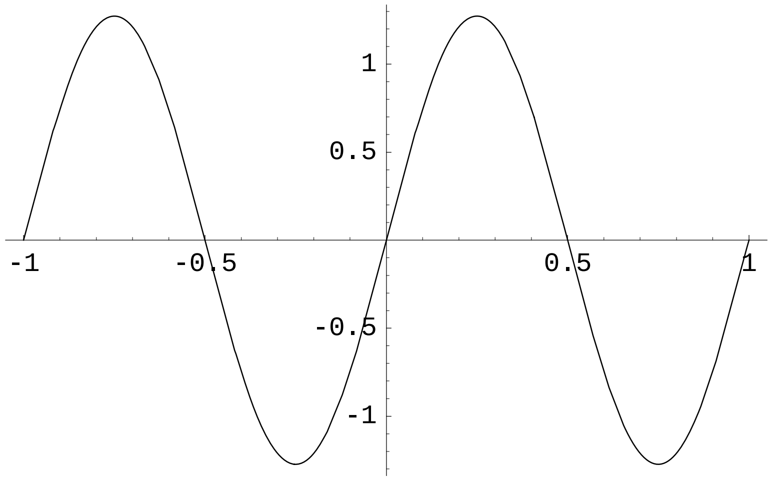


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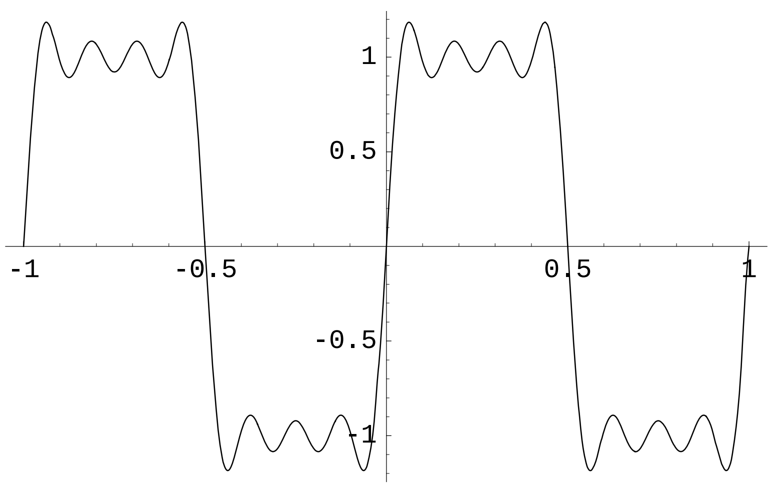
Plot[f[x, 1] + f[x, 3] + f[x, 5] + f[x, 7], {x, -1., 1.}]
```

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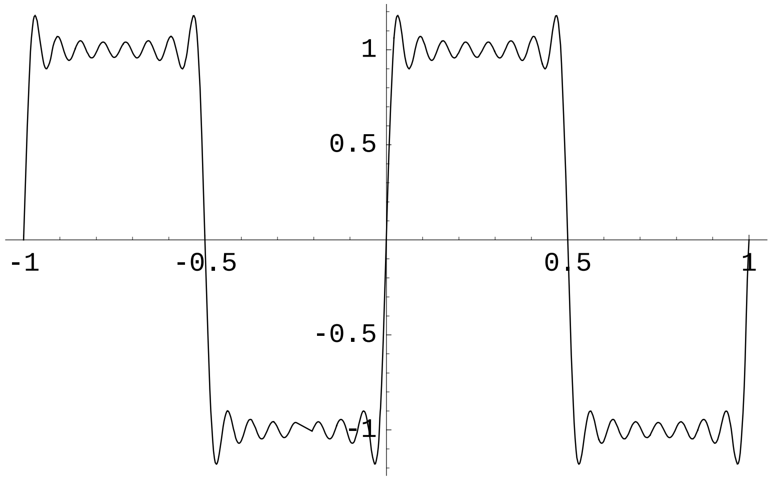
```
Plot[f[x, 1] + f[x, 3] + f[x, 5] + f[x, 7] +
  f[x, 9] + f[x, 11] + f[x, 13] + f[x, 15], {x, -1., 1.}]
```

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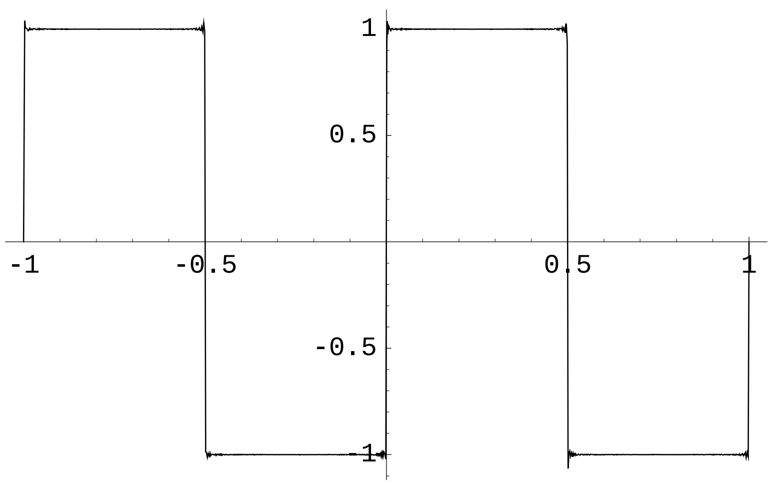
Plot[Sum[f[x, i], {i, 1, 1000, 2}], {x, -1., 1.}]
```

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Continuous sets of eigenfunctions and the dirac delta function

OK, we defined functions over the interval -L/2 to L/2. What happens if we want to look at functions defined between -∞ and ∞?

We will have to introduce a new set of basis vectors (or eigenfunctions or later eigenkets) which are not discreet, but are continuous. Not only are there an infinite number of them, there are an infinite number in any finite interval. We rewrite the sum

$$f(x)=\sum_{n=0}^{\infty}\left[a_n\sqrt{\frac{2}{L}}\cos\frac{2\,n\pi x}{L}+b_n\sqrt{\frac{2}{L}}\sin\frac{2\,n\pi x}{L}\right]$$

$$\text{as } f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)\,e^{ikx}\,dk \tag{4}$$

Note that the sum over n has become an integral over k, the coefficients a_n and b_n have become a function A(k) and the sines and cosines have been replaced by e^{ikx}. It turns out that over the interval -∞ to ∞ the functions e^{ikx} form a set of orthonormal functions that can be used as the basis functions. I am not going to prove this but I will only write down the answers because I will spend most of my time on the continuous form of the δ function - the Dirac delta function.

So we have

$$\begin{gathered} f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)\,e^{ikx}\,dk \\ \text{and } A(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)\,e^{-ikx}\,dx \qquad \text{[the fourier integral transformation]} \end{gathered} \tag{5}$$

Now lets write out the orthogonality condition for the e^{ikx}'s

$\int_{-\infty}^{\infty}\phi^*(x)\,\phi(x)\,dx$ =

some sort of delta function where the ϕ's refer to the e^{ikx}'s. When functions are complex we take the complex conjugate. For the sin's and cos's it wouldnt' have mattered thought tehcnically you could put the * in all the eqn's.

The condition is $\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}\,e^{-ikx'}\,dk=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ik(x-x')}dk=\delta(x-x')$

Loosely speaking the dirac delta function $\delta(x-x_0)=0$ if $x\neq x_0$ and has a spike at $x=x_0$

It is normalized such that $1=\int_{-\infty}^{\infty}\delta(x-x_0)dx$

The δ function only has meaning under an integral.

This now means

f(x)=$\int f(x') \, \delta(x - x') \, \mathrm{dx}'$

[often we leave out the limits since it clear we will mean the limit over the entire region of interest]

there are more important characteristics of delta functions that you will need which you will learn as part of the problem set.

