Dirac delta function in terms of orthogonal functions.

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March 8, 2009. Last Revision: $Date : 2009/03/1003 : 20 : 36$

1 Motivation.

Chapter II of [Pauli(2000)] expresses the delta function in terms of orthonormal basis functions, but the treatment is slightly hard to follow. Reexpress some of this in my own words the slow and dumb way to get an understanding of the ideas. Also explore the summation representation of the delta function and use it to relate Fourier series and transforms.

2 Fourier coefficients.

Given an orthonormal basis

$$\int u_m^*(x) u_n(x) = \delta_{mn}$$

For a function that can be expressed entirely in this basis, such as

$$f(x) = \sum_k a_k u_k(x)$$

We can then compute the Fourier coefficients a_k in the normal fashion

$$\begin{aligned}\int u_k^*(x) f(x) dx &= \sum_n a_n \int u_k^*(x) u_n(x) dx \\ &= \sum_n a_n \delta_{kn} \\ &= a_k\end{aligned}$$

So we have

$$f(x) = \sum_k a_k u_k(x) = \sum_k u_k(x) \int u_k^*(x') f(x') dx'$$

2.1 Mean square convergence.

How good of a match is a subset of such a sum? Pauli considers a mean convergence.

$$
\begin{aligned}
0 &= \lim_{N\to\infty} \int \left| f(x') - \sum_{k=1}^{N} a_k u_k(x') \right|^2 dx' \\
&= \int \left(f^*(x') - \sum_{k=1}^{N} a_k^* u_k^*(x') \right) \left(f(x') - \sum_{m=1}^{N} a_m u_m(x') \right) dx' \\
&= \int \left(f^*(x') f(x') - f^*(x') \sum_{m=1}^{N} a_m u_m(x') - \sum_{k=1}^{N} a_k^* u_k^*(x') f(x') + \sum_{m=1}^{N} a_m u_m(x') \sum_{k=1}^{N} a_k^* u_k^*(x') \right) dx' \\
&= \int f^*(x') f(x') dx' - \sum_{m=1}^{N} a_m a_m^* - \sum_{k=1}^{N} a_k^* a_k + \sum_{m=1}^{N} \sum_{k=1}^{N} a_m a_k^* \delta_{km} \\
&= \int \left| f(x') \right|^2 dx' - \sum_{m=1}^{N} |a_m|^2
\end{aligned}
$$

So if we have mean square equality in the limit as $N \to \infty$, then it must also be true that

$$
\int \left| f(x') \right|^2 dx' = \sum_{m=1}^{\infty} |a_m|^2
$$

He calls this the completeness relation. If the orthonormal basis is sufficient to express the set of desired functions, then the squared absolute value of such functions can be expressed entirely in terms of the fourier coefficients. The mean square equality is weaker in the sense that a function can be mismatched to its fourier representation at a set (of "measure zero") points, and still meet the mean square equality statement.

2.2 Generalizing the inner product.

Pauli next introduces the an inner product on functions (without calling it that) in a somewhat indirect fashion (ie: in terms of fourier components instead of by definition).

Supposing that one has two functions built up by Fourier components

$$
\begin{aligned}
f(x) &= \sum_k a_k u_k(x) \\
g(x) &= \sum_k b_k u_k(x)
\end{aligned}
$$

Then we have

$$\int f^*(x)g(x) = \sum_{k,m} a_k^* b_m \int u_k^*(x)u_m(x) = \sum_k a_k^* b_k$$
$$\int g^*(x)f(x) = \sum_{k,m} a_k b_m^* \int u_m^*(x)u_k(x) = \sum_k b_k^* a_k$$

This is something that is familar to anybody who has taken a linear algebra course, but perhaps had to be motivated when he wrote the book?

2.3 Delta function as a sum.

Perhaps Pauli wrote this general function inner product that way to show a natural way that a sum of the form

$$\sum u_m^*(x)u_k(x)$$

arises in use, because he now writes the completeness relation using a sum similar to that above

$$\sum_k u_k^*(x')u_k(x) \equiv \delta(x - x') \tag{1}$$

I'd seen this in bra ket notation, in Susskind's lectures as noted in [Joot()], and also in [McMahon(2005)] as the identity operator

$$\sum_k |k\rangle\langle k| \equiv \delta(x - x') \tag{2}$$

From neither of those two sources did I understand where it came from (in Susskind's lectures it appeared to be related to Fourier transforms). As Pauli did, let's verify that this works, and try to relate this to a few specific choices of inner products (covering at least classical Fourier series and the Fourier transform).

The relation of equation 1 can be shown to have delta function behaviour by integration

$$\begin{aligned}
\int \sum_k u_k^*(x')u_k(x)f(x')dx' &= \sum_{k,m} u_k(x)a_m \int u_k^*(x')u_m(x')dx' \\
&= \sum_{k,m} u_k(x)a_m\delta_{km} \\
&= \sum_k u_k(x)a_k \\
&= f(x)
\end{aligned}$$

Strictly speaking this ought to be formulated in terms of mean square convergence since an arbitrary function f(x) may differ from its Fourier sum at specific points (for example at points of discontinuity).

2.3.1 Fourier series example.

Suppose the inner product is defined for the range $I = [a, a+T]$.

$$\langle f, g \rangle = \int_{\partial I} f^*(x) g(x) dx$$

What is the identity operator representation in the Fourier series basis $u'_k(x) = e^{2\pi i k x/T}$? First the normalization is required.

$$\begin{aligned}\langle u'_k, u'_m \rangle &= \int_{\partial I} e^{2\pi i (m-k) x/T} dx \\ &= \delta_{km} T\end{aligned}$$

So our orthonormalized basis is

$$u_k(x) = \frac{1}{\sqrt{T}} e^{2\pi i k x/T}$$

Given this orthonormal basis we can write

$$\begin{aligned}f(x) &= \sum_k a_k u_k(x) \\ a_k &= \int_{\partial I} u_k^*(x) f(x) dx = \langle u_k(x), f(x) \rangle\end{aligned}$$

Or in a vector like notation

$$f(x) = \sum_k u_k(x) \langle u_k(x), f(x) \rangle$$

In this basis the delta function (identity operator) form of equation 1 becomes

$$\delta(x - x') = \frac{1}{T} \sum_k e^{2\pi i k (x - x')/T}$$

2.3.2 Fourier transform innerproduct.

For the Fourier transform we have an infinite range inner product

$$\langle f, g \rangle = \int_{-\infty}^{\infty} f^*(x) g(x) dx$$

With a fourier transform pair

$$\begin{aligned}
\hat{f}(k) &= \frac{1}{\sqrt{2\pi}} \int f(x) e^{-ikx} dx \\
f(x) &= \frac{1}{\sqrt{2\pi}} \int \hat{f}(k) e^{ikx} dk
\end{aligned}$$

It appears that a natural choice of basis functions is actually u_k from the Fourier series above with $T = 2\pi$. That is

$$u_k = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

Our fourier coefficients are now continuous and we have a form that is very close to the discrete fourier series

$$\begin{aligned}
f(x) &= \int dk a_k u_k \\
a_k &= \int u_k^*(x) f(x) dx = \langle u_k(x), f(x) \rangle
\end{aligned}$$

Besides the inner product range difference from the discrete frequency case the only other difference in this formulation is that we have a $\sum_k \rightarrow \int dk$ replacement.

What is the delta function representation in this inner product space?

A continuous variation of the summation delta function representation in the Fourier series basis is

$$\int dk u_k^*(x) u_k(x') = \int dk \frac{1}{2\pi} e^{ik(x'-x)}$$

Okay, cool. The principle value of this integral is the sinc function that is the familiar limiting form of the delta function.

This is an interesting and unifying way of expressing these Fourier relationships. The inner product is seen here to provide a more general structure that is common to both the Fourier series and Fourier transform. It isn't suprising that the physicists rightly pick the algebraic orthonormal function representation as fundamental ... too bad they do it all with the braket notation that automatically obfuscates the subject.

This also clarifies for me what Susskind did in his QM lectures. There he used the identity operator representation to express the Fourier transform without ever touching on the tricky aspects of Fourier inversion. That's a tricky but interesting approach.

2.3.3 Legendre polynomials

Let's see how one non-Fourier like inner product function space representation works out this way.

Using the Legrendre inner product

$$\langle f, g \rangle = \int_{-1}^{1} f(x) g(x) dx$$

An orthonormal basis can be had by normalizing the Legendre polynomials. Wolfram's Legendre Polynomial page lists these in a number of closed forms

$$\begin{aligned} P_n(x) &= \frac{1}{2\pi i} \oint \frac{dt}{t^{n+1} \sqrt{1 - 2tx + t^2}} \\ &= \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k}^2 (x-1)^{n-k} (x+1)^k \end{aligned}$$

The first of these uses a closed contour around the origin.

These polynomials aren't orthonormal, having

$$\langle P_n, P_m \rangle = \frac{2}{2n+1} \delta_{mn}$$

So we have an orthonormal basis if we pick

$$u_n(x) = P_n(x) \sqrt{n + 1/2}$$

Our delta function representation in this basis becomes

$$\begin{aligned} \delta(x - x') &\sim \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) P_n(x') P_n(x) \\ &= -\frac{1}{4\pi^2} \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) \oint \frac{du}{u^{n+1} \sqrt{1 - 2ux' + u^2}} \oint \frac{dt}{t^{n+1} \sqrt{1 - 2tx + t^2}} \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{k=0}^{n} \frac{n + \frac{1}{2}}{2^{2n}} \binom{n}{m}^2 (x'-1)^{n-m} (x'+1)^m \binom{n}{k}^2 (x-1)^{n-k} (x+1)^k \end{aligned}$$

Neither of these are familiar looking to me, but I was mostly curious to see one of these delta representations for a non-Fourier-ish basis. A number of other orthogonal polynomials can be found detailed in Wolfram's orthogonal polynomial article.

References

[Joot()] Peeter Joot. Notes on susskind's qm lectures. "http://sites.google.com/site/peeterjoot/math2009/qm_susskind.pdf".

[McMahon(2005)] D. McMahon. *Quantum Mechanics Demystified*. McGraw-Hill Professional, 2005.

[Pauli(2000)] W. Pauli. *Wave Mechanics*. Courier Dover Publications, 2000.