VECTOR SPACES AND HILBERT SPACE

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Section 3.1; Problem 3.1.

We've looked at a lot of examples of wave functions for various potentials, and one thing we have demanded of all of them is that they are *normalizable*, that is, that

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

Although we can (rightly) look at $\psi(x)$ as an ordinary function (albeit a complex one), it is also possible to regard it as a *vector*. The common conception of a vector is an arrow in two- or three-dimensional space, with coordinates in each of the spatial directions, such as $\mathbf{r} = [1, -2, 4]$. However, it is possible to generalize the idea of a vector so that it possesses any number of dimensions, and in fact, we can extend this notion to vectors that have an infinite number of dimensions.

Looked at this way, $\psi(x)$ is a vector with a value or component for every value of x.

A set of vectors can form a *vector space* if it satisfies two conditions:

(1) If a vector $\psi_1(x)$ is in the set, then so is $A\psi_1(x)$ for any complex scalar A.
(2) If two vectors $\psi_1(x)$ and $\psi_2(x)$ are in the set, then so is their sum $\psi_1(x) + \psi_2(x)$.

These two conditions can be combined by saying that if two vectors $\psi_1(x)$ and $\psi_2(x)$ are in the set, then so is their *linear combination* $A\psi_1(x) + B\psi_2(x)$, for any complex scalars A and B.

From this definition, we can show that the set of all normalizable functions referred to above is *not* in fact a vector space. For example, if 1 is true for a vector $\psi(x)$, then it is not true if we multiply $\psi(x)$ by any scalar A where $|A| \neq 1$.

However, if we consider the super-set of vectors that are required only to be *square-integrable*, that is, that satisfy the requirement that $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx$ is *finite*, but not necessarily 1, then this set *is* a vector space.

To show this, it's easier if we introduce a shorthand notation. The integral 1 is an example of an *inner product* (essentially a generalization of the dot or scalar product for finite-dimensional vectors). In general, the inner product of two vectors is

$$\langle f|g\rangle \equiv \int_{-\infty}^{\infty} f^*(x)g(x)dx \tag{2}$$

(The limits on the integral don't have to be infinite if we're considering functions defined over some other, possibly finite, interval.)

From the definition of a vector space, a set of functions must be closed under addition and scalar multiplication to qualify. For the set of all square-integrable functions, clearly scalar multiplication of any function by a finite value does not affect its square-integrable nature. For the sum, consider two functions f and g from the set. By assumption, $\langle f|f\rangle$and $\langle g|g\rangle$ are finite, so we must show that $\langle f+g|f+g\rangle$ is finite as well. We have

$$\langle f+g|f+g\rangle = \langle f|f\rangle + \langle f|g\rangle + \langle g|f\rangle + \langle g|g\rangle \tag{3}$$

At this point, we need to introduce a theorem known as the Schwartz inequality. For any two square-integrable functions, the theorem says that

$$|\langle f|g\rangle|^2 \le \langle f|f\rangle \langle g|g\rangle \tag{4}$$

(Note that the right-hand side here is always real, since the inner product of a function with itself multiplies the function by its complex conjugate inside the integral.)

From the Schwartz inequality, we know that both $\langle f|g\rangle$ and $\langle g|f\rangle$ are bounded by $\sqrt{\langle f|f\rangle \langle g|g\rangle}$, which is finite by assumption, so the set of square-integrable functions is closed under addition and is a vector space.

In physics, this vector space is known as *Hilbert space*, named after the German mathematician David Hilbert (1862-1943). The set of normalizable functions is a subset of Hilbert space, but is not itself a vector space, as we've already seen.

More generally, the mathematical definition of an inner product of two vectors requires that it satisfies three conditions:

(1) $\langle g|f\rangle = \langle f|g\rangle^*$
(2) $\langle f|f\rangle \ge 0$ and $\langle f|f\rangle = 0$ if and only if $|f\rangle = 0$ (that is, in function notation, $f(x) = 0$ for all x).
(3) $\langle h|(A|f\rangle + B|g\rangle) = A\langle h|f\rangle + B\langle h|g\rangle$

The definition of the inner product in terms of the integral 2 above satisfies these three conditions. First

$$\langle g|f\rangle = \langle f|g\rangle^* \tag{5}$$

This is obviously true from the definition

Second $\langle f|f\rangle \geq 0$, with $\langle f|f\rangle = 0$ iff $|f\rangle = |0\rangle$. Again, using 2, we must have $\langle f|f\rangle \geq 0$, since we are integrating the square modulus of a complex function, which is non-negative everywhere. We also must have $\langle f|f\rangle = 0$ iff $|f\rangle = |0\rangle$ since if $|f\rangle \neq |0\rangle$ anywhere, then the integral would have a positive contribution. Conversely the only way the integral of a non-negative function can be zero is for the function to be zero everywhere. (We are ignoring pathological functions that are non-zero at isolated points since these cannot represent physical systems.)

Finally, the third condition for an inner product is again fairly obvious from the definition:

$$\begin{aligned}
\langle h|\left(A|f\rangle + B|g\rangle\right) &= \int_{-\infty}^{\infty} \left[h^*(x)Af(x) + h^*(x)Bg(x)\right]dx && (6)\\
&= \int_{-\infty}^{\infty} h^*(x)Af(x)dx + \int_{-\infty}^{\infty} h^*(x)Bg(x)dx && (7)\\
&= A\int_{-\infty}^{\infty} h^*(x)f(x)dx + B\int_{-\infty}^{\infty} h^*(x)g(x)dx && (8)\\
&= A\langle h|f\rangle + B\langle h|g\rangle && (9)
\end{aligned}$$

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