HERMITIAN OPERATORS

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Reference: Arfken, George B. & Weber, Hans J. (2005), Mathematical Methods for Physicists, 6th Edition, Academic Press - Sec 10.2.

We saw in the last post that a second-order ODE in the form

$$p_0(x)u'' + p_1(x)u' + p_2(x)u + \lambda w(x)u(x) = 0 \tag{1}$$

is self-adjoint if

$$p_0' = p_1 \tag{2}$$

and that any second-order ODE can be transformed into self-adjoint form by multiplying through by the correct function.

A self-adjoint operator L can be written as

$$Lu = (p_0 u')' + p_2 u \tag{3}$$

If we multiply this operator by the complex conjugate of another function $v(x)$, and then integrate between two limits a and b, we get

$$\int_a^b v^* Lu\,dx = \int_a^b v^*(p_0 u')'\,dx + \int_a^b v^* p_2 u\,dx \tag{4}$$

The first integral on the right can be integrated by parts twice to get

$$\begin{aligned}\int_a^b v^*(p_0u')'\,dx &= v^* p_0 u\Big|_a^b - \int_a^b (v^*)' p_0 u'\,dx &(5)\\ &= v^* p_0 u\Big|_a^b - (v^*)' p_0 u\Big|_a^b + \int_a^b u(p_0(v^*)')'\,dx &(6)\end{aligned}$$

If the two integrated terms in the last line vanish due to satisfying boundary conditions

$$v^* p_0 u\Big|_a = v^* p_0 u\Big|_b \tag{7}$$

and

$$(v^*)' p_0 u\Big|_a = (v^*)' p_0 u\Big|_b \tag{8}$$

then we get the condition

$$\int_a^b v^* L u \, dx = \int_a^b u (L v)^* \, dx \tag{9}$$

An operator L that satisfies this condition is called *Hermitian*. Note that the condition applies for *any* functions u and v; these functions do not have to be solutions of any particular ODE. What they *do* have to do is satisfy the boundary conditions above.

Note that in this derivation, we've assumed that L is a real, second-order differential operator. Although such operators frequently turn up in physics, especially in quantum mechanics, the condition can be generalized to operators that are not necessarily second-order or real. So a general, possibly complex, differential operator L that satisfies 9 is called Hermitian, and the derivation above should be seen as a special case of one class of operators that happen to be Hermitian. Another example which is not a second-order operator or real is the quantum mechanical momentum operator $p = -i\hbar\partial/\partial x$.

For this operator, the above equation is

$$\int_a^b v^* L u \, dx = -i\hbar \int_a^b v^* \frac{d}{dx} u \, dx \tag{10}$$

Integrating by parts gives us

$$-i\hbar \int_a^b v^* \frac{du}{dx} \, dx = -i\hbar v^* u \Big|_a^b + i\hbar \int_a^b u \frac{dv^*}{dx} dx \tag{11}$$

If we choose the limits $a = -\infty$ and $b = +\infty$, then we are justified in taking both u and v to be zero at the limits in order that these functions are normalizable, as is required in quantum mechanics. Thus the integrated term is zero, and we are left with

$$-i\hbar \int_a^b v^* \frac{du}{dx} \, dx = i\hbar \int_a^b u \frac{dv^*}{dx} dx \tag{12}$$

or, in terms of the momentum operator p

$$\int_{-\infty}^{\infty} v^* p u \, dx = \int_{-\infty}^{\infty} (p v)^* u \, dx \tag{13}$$

which is precisely the Hermitian condition. Note that the fact that p is complex, due to the i in its definition, is essential for it to be Hermitian, since the negative sign that arises in the integration by parts translates into the $-i$ in the original operator becoming a $+i$ in the complex conjugate.

Now suppose we consider the ODE

$$Lu_i(x) + \lambda_i w(x) u_i(x) = 0 \tag{14}$$

where λ_i is a constant called the *eigenvalue* and $w(x)$ is another function (assumed to be real and positive) of x known as the *weighting function*. The subscript i labels a particular solution of this ODE, so that a given solution u_i is associated with a particular eigenvalue λ_i.

For another solution u_j we can take the complex conjugate of 14 to get

$$L^* u_j^*(x) + \lambda_j^* w(x) u_j^*(x) = 0 \tag{15}$$

We can multiply 14 by u_j^* and 15 by u_i, integrate between limits a and b such that the boundary conditions above are satisfied (Such boundary conditions usually exist in quantum mechanics. For example, in a one-dimensional problem with a potential of infinite range (such as the harmonic oscillator) if $a = -\infty$ and $b = +\infty$, the wave function is required to be zero at both limits in order for it to be normalizable.) and then take the difference we get:

$$\int_a^b u_j^* L u_i \, dx - \int_a^b u_i L^* u_j^* \, dx = (\lambda_j^* - \lambda_i) \int_a^b u_i u_j^* w \, dx \tag{16}$$

If L is Hermitian, the left-hand side of this equation is zero. This leads to two important results. First, if $i = j$, then provided we assume that neither u_i nor w are zero everywhere, the integral on the right must be non-zero. Therefore we get

$$\lambda_i^* = \lambda_i \tag{17}$$

In other words, the eigenvalues of a Hermitian operator are real. This has a physical interpretation in quantum mechanics, since every quantity representable by a Hermitian operator should be observable.

The other consequence is that if $i \neq j$, then if the eigenvalues for distinct solutions are different, the integral on the right must be zero. That is

$$\int_a^b u_i u_j^* w \, dx = 0 \tag{18}$$

if $i \neq j$. This condition means that the distinct solutions of 14 are *orthogonal* functions. Note however that the orthogonality condition may require a weighting function in order for the integral to be zero. In fact, many of the functions encountered in quantum mechanics have $w(x) \equiv 1$, but there are some notable exceptions such as Laguerre and Hermite polynomials.

We haven't dealt with the case of *degenerate* eigenvalues, that is, cases where distinct solutions u_i and u_j have the same eigenvalue, but that's a topic for another post.

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