

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

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

is self-adjoint if

$$(2) \quad p_0' = p_1$$

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

$$(3) \quad Lu = (p_0u')' + p_2u$$

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

$$(4) \quad \int_a^b v^* Lu \, dx = \int_a^b v^* (p_0u')' \, dx + \int_a^b v^* p_2u \, dx$$

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

$$(5) \quad \int_a^b v^* (p_0u')' \, dx = v^* p_0u \Big|_a^b - \int_a^b (v^*)' p_0u' \, dx$$

$$(6) \quad = v^* p_0u \Big|_a^b - (v^*)' p_0u \Big|_a^b + \int_a^b u (p_0(v^*)')' \, dx$$

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

$$(7) \quad v^* p_0u \Big|_a = v^* p_0u \Big|_b$$

and

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

then we get the condition

$$(9) \quad \int_a^b v^* L u \, dx = \int_a^b u (L v)^* \, dx$$

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

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

Integrating by parts gives us

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

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

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

or, in terms of the momentum operator p

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

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

$$(14) \quad L u_i(x) + \lambda_i w(x) u_i(x) = 0$$

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

$$(15) \quad L^* u_j^*(x) + \lambda_j^* w(x) u_j^*(x) = 0$$

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:

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

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

$$(17) \quad \lambda_i^* = \lambda_i$$

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

$$(18) \quad \int_a^b u_i u_j^* w dx = 0$$

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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