

## 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

$$(0.1) \quad p_0(x)u'' + p_1(x)u' + p_2(x)u + \lambda w(x)u(x) = 0$$

is self-adjoint if

$$(0.2) \quad p_0' = p_1$$

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

$$(0.3) \quad Lu = (p_0u')' + p_2u$$

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

$$(0.4) \quad \int_a^b v^* Lu \, dx = \int_a^b v^* (p_0u')' \, dx + \int_a^b v^* p_2u \, dx$$

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

$$(0.5) \quad \int_a^b v^* (p_0u')' \, dx = v^* p_0u \Big|_a^b - \int_a^b (v^*)' p_0u' \, dx$$

$$(0.6) \quad = v^* p_0u \Big|_a^b - (v^*)' p_0u \Big|_a^b + \int_a^b u (p_0(v^*)')' \, dx$$

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

$$(0.7) \quad v^* p_0u \Big|_a = v^* p_0u \Big|_b$$

and

$$(0.8) \quad (v^*)' p_0 u \Big|_a = (v^*)' p_0 u \Big|_b$$

then we get the condition

$$(0.9) \quad \int_a^b v^* L u \, dx = \int_a^b u (L v)^* \, dx$$

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 0.9 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

$$(0.10) \quad \int_a^b v^* L u \, dx = -i\hbar \int_a^b v^* \frac{d}{dx} u \, dx$$

Integrating by parts gives us

$$(0.11) \quad -i\hbar \int_a^b v^* \frac{du}{dx} \, dx = -i\hbar v^* u \Big|_a^b + i\hbar \int_a^b u \frac{dv^*}{dx} \, dx$$

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

$$(0.12) \quad -i\hbar \int_a^b v^* \frac{du}{dx} \, dx = i\hbar \int_a^b u \frac{dv^*}{dx} \, dx$$

or, in terms of the momentum operator  $p$

$$(0.13) \quad \int_{-\infty}^{\infty} v^* p u \, dx = \int_{-\infty}^{\infty} (p v)^* u \, dx$$

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

$$(0.14) \quad L u_i(x) + \lambda_i w(x) u_i(x) = 0$$

where  $\lambda_i$  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  $\lambda_i$ .

For another solution  $u_j$  we can take the complex conjugate of 0.14 to get

$$(0.15) \quad L^* u_j^*(x) + \lambda_j^* w(x) u_j^*(x) = 0$$

We can multiply 0.14 by  $u_j^*$  and 0.15 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:

$$(0.16) \quad \int_a^b u_j^* L u_i \, dx - \int_a^b u_i L^* u_j^* \, dx = (\lambda_j^* - \lambda_i) \int_a^b u_i u_j^* w \, dx$$

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

$$(0.17) \quad \lambda_i^* = \lambda_i$$

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

$$(0.18) \quad \int_a^b u_i u_j^* w dx = 0$$

if  $i \neq j$ . This condition means that the distinct solutions of 0.14 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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