Dr. F. Amar

Chy 475
Spring 2009

Hermitian operators

Physical observables are represented by hermitian operators and hermitian operators have real eigenvalues.

Physical observables whose values can be measured have values that are real scalar quantities (not complex numbers). This means that

$$\langle A \rangle = \int_{-\infty}^{+\infty} \psi^*(x)\hat{A}\psi(x)dx \qquad (1)$$

is a real number. This in turn implies that <A>=<A>* or that

$$\int_{-\infty}^{+\infty} \psi^*(x)\hat{A}\psi(x)dx = \left\{ \int_{-\infty}^{+\infty} \psi^*(x)\hat{A}\psi(x)dx \right\}^* \qquad (2)$$

What does it mean to take the complex conjugate of the whole integral expression? Basically we have to turn every $+i$ into $-i$ in the expression which leads to:

$$\int_{-\infty}^{+\infty} \psi^*(x)\hat{A}\psi(x)dx = \int_{-\infty}^{+\infty} \psi(x)\hat{A}^*\psi^*(x)dx \qquad (3)$$

An operator, $\hat{A}$, that satisfies eqn. 3, or more generally, eqn. 4:

$$\int_{-\infty}^{+\infty} f^*(x)\hat{A}g(x)dx \int_{-\infty}^{+\infty} g(x)\hat{A}^* f^*(x)dx, \qquad (4)$$

is *a Hermitian operator*. So we've shown that real eigenvalues imply that the operator is Hermitian. What about the converse. if eqn (4) is obeyed, will the eigenvalues of $\hat{A}$ be real?

Proof: Suppose that we apply eqn 4 in the situation where f and g are the same function and f is an eigenfunction of $\hat{A}$ with eigenvalue b. Then we have:

$$\int_{-\infty}^{+\infty} f^*\hat{A}f dx = \int_{-\infty}^{+\infty} f\hat{A}^* f^* dx, \qquad (5)$$

The eigenfunction-eigenvalue relationship can be written,

$$\hat{A}\ f = bf \qquad (6)$$

Taking the complex conjugate of both sides of this equation we see that

$$\hat{A}^* f^* = b^* f^* \qquad (7)$$

Now let us plug (6) and (7) into (5):

$$\int_{-\infty}^{+\infty} f^* bf dx = \int_{-\infty}^{+\infty} f b^* f^* dx \quad \text{or} \quad b\int_{-\infty}^{+\infty} f^* f dx = b^* \int_{-\infty}^{+\infty} f f^* dx \qquad (8)$$

Since $\int_{-\infty}^{+\infty} f^* f dx = \int_{-\infty}^{+\infty} f f^* dx = \int_{-\infty}^{+\infty} |f|^2 dx > 0,$

we have the situation that the fact that the operator is Hermitian implies that $b=b^*$. But if $b=b^*$ then b (the eigenvalue) is real. QED

Eigenfunctions of a Hermitian operator that correspond to different eigenvalues are orthogonal [*in the square-integrable sense*]

Proof: Suppose that *f* and *g* different eigenfunctions of the Hermitian operator $\hat{A}$ with <u>different</u> eigenvalues *b and c respectively*. Then the Hermitian property (eqn 4) is

$$\int_{-\infty}^{+\infty} g^* \hat{A} f dx = \int_{-\infty}^{+\infty} f \hat{A}^* g^* dx, \qquad (9)$$

The necessary eigenfunction-eigenvalue relationships can be written,

$$\hat{A}\ f = bf\ ;\ \hat{A}\ g = cg \quad \rightarrow \quad \hat{A}^* g^* = c^* g^* = cg^* \qquad (10)$$

Now let us plug relationships from (10) into (9):

$$\int_{-\infty}^{+\infty} g^* bf dx = \int_{-\infty}^{+\infty} f c g^* dx \qquad \text{or} \qquad (11)$$

$$b\int_{-\infty}^{+\infty} g^* f dx = c\int_{-\infty}^{+\infty} f g^* dx \ = c\int_{-\infty}^{+\infty} g^* f dx \qquad (12)$$

which can be rearranged to give:

$$(b-c)\int_{-\infty}^{+\infty} g^* f dx = 0 \qquad (13)$$

Since (b-c) ≠ 0 then $\int_{-\infty}^{+\infty} g^* f dx = 0$ must be true, but this IS the orthogonality condition. QED.

The eigenfunctions of a Hermitian operator form a complete set.

A set of functions, $\{f\}$, defined on some interval such as [0,1] or (-∞,+∞) is a complete set if any well-behaved function, g, on the interval can be written as a linear combination of the functions:

$$g(x) = \sum_i c_i f_i(x)$$

We say that *g(x)* is expanded in terms of the *f*s.

Mathematicians have shown that the trigonometric functions {sin(nπx), n=1,2,3,…} form a complete set for the interval [0,1]. The series expansion of this kind is called a Fourier series. Similarly, the eigenfunctions of the harmonic oscillator Hamiltonian (which is a Hermitian operator) are a complete set on the interval (-∞,+∞)

The fact that the functions $\{f\}$ are eigenfunctions of Hermitian operators means that they are normalized and orthogonal already and we can use these properties to find the expansion coefficients, c_i.

Start with $g = \sum_i c_i f_i$

Multiply g from the left by f_k*: $f_k^* g = f_k^* \sum_i c_i f_i$

and then integrate the resulting function over all space:

$$\int f_k^* g dx = \int f_k^* \sum_i c_i f_i dx = \sum_i \int f_k^* c_i f_i dx = \sum_i c_i \int f_k^* f_i dx = \sum_i c_i \delta_{ki} = c_k.$$

Thus: $c_k = \int f_k^* g dx$ where f_k is one of the known eigenfunctions and g is the arbitrary function we want to expand in the complete set.