11.2: Improved Notation

Before commencing our investigation, it is helpful to introduce some improved notation. Let the ψ_i be a complete set of eigenstates of the Hamiltonian, H, corresponding to the eigenvalues E_i: that is,

$$H\,\psi_i = E_i\,\psi_i. \tag{11.2.1}$$

Now, we expect the ψ_i to be orthonormal. (See Section [seig].) In one dimension, this implies that

$$\int_{-\infty}^{\infty}\psi_i^\ast\,\psi_j\,dx = \delta_{ij}. \tag{11.2.2}$$

In three dimensions (see Chapter [sthree]), the previous expression generalizes to

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_i^\ast\,\psi_j\,dx\,dy\,dz = \delta_{ij}. \tag{11.2.3}$$

Finally, if the ψ_i are spinors (see Chapter [sspin]) then we have

$$\psi_i^\dagger\,\psi_j = \delta_{ij}. \tag{11.2.4}$$

The generalization to the case where ψ is a product of a regular wavefunction and a spinor is fairly obvious. We can represent all of the previous possibilities by writing

$$\langle\psi_i|\psi_j\rangle \equiv \langle i|j\rangle = \delta_{ij}. \tag{11.2.5}$$

Here, the term in angle brackets represents the integrals appearing in Equations ([e12.1]) and ([e12.2]) in one- and three-dimensional regular space, respectively, and the spinor product appearing in Equation ([e12.3]) in spin-space. The advantage of our new notation is its great generality: that is, it can deal with one-dimensional wavefunctions, three-dimensional wavefunctions, spinors, et cetera.

Expanding a general wavefunction, ψ_a, in terms of the energy eigenstates, ψ_i, we obtain

$$\psi_a = \sum_i c_i\,\psi_i. \tag{11.2.6}$$

In one dimension, the expansion coefficients take the form (see Section [seig])

$$c_i = \int_{-\infty}^{\infty}\psi_i^\ast\,\psi_a\,dx, \tag{11.2.7}$$

whereas in three dimensions we get

$$c_i = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_i^\ast\,\psi_a\,dx\,dy\,dz. \tag{11.2.8}$$

Finally, if ψ is a spinor then we have

$$c_i = \psi_i^\dagger\,\psi_a. \tag{11.2.9}$$

We can represent all of the previous possibilities by writing

$$c_i = \langle\psi_i|\psi_a\rangle \equiv \langle i|a\rangle. \tag{11.2.10}$$

The expansion ([e12.7]) thus becomes

$$\psi_a = \sum_i\langle\psi_i|\psi_a\rangle\,\psi_i \equiv \sum_i\langle i|a\rangle\,\psi_i. \tag{11.2.11}$$

Incidentally, it follows that

$$\langle i|a\rangle^\ast = \langle a|i\rangle. \tag{11.2.12}$$

Finally, if A is a general operator, and the wavefunction ψ_a is expanded in the manner shown in Equation ([e12.7]), then the expectation value of A is written (see Section [seig])

$$\langle A\rangle = \sum_{i,j} c_i^\ast\, c_j\, A_{ij}. \tag{11.2.13}$$

Here, the A_{ij} are unsurprisingly known as the *matrix elements* of A. In one dimension, the matrix elements take the form

$$A_{ij} = \int_{-\infty}^{\infty} \psi_i^\ast\, A\,\psi_j\, dx, \tag{11.2.14}$$

whereas in three dimensions we get

$$A_{ij} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_i^\ast\, A\,\psi_j\, dx\, dy\, dz. \tag{11.2.15}$$

Finally, if ψ is a spinor then we have

$$A_{ij} = \psi_i^\dagger\, A\,\psi_j. \tag{11.2.16}$$

We can represent all of the previous possibilities by writing

$$A_{ij} = \langle\psi_i|A|\psi_j\rangle \equiv \langle i|A|j\rangle. \tag{11.2.17}$$

The expansion ([e12.14]) thus becomes

$$\langle A\rangle \equiv \langle a|A|a\rangle = \sum_{i,j}\langle a|i\rangle\langle i|A|j\rangle\langle j|a\rangle. \tag{11.2.18}$$

Incidentally, it follows that [see Equation ([e5.48])]

$$\langle i|A|j\rangle^\ast = \langle j|A^\dagger|i\rangle. \tag{11.2.19}$$

Finally, it is clear from Equation ([e12.20a]) that

$$\sum_i |i\rangle\langle i| \equiv 1, \tag{11.2.20}$$

where the ψ_i are a complete set of eigenstates, and 1 is the identity operator.

Contributors and Attributions

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