from **Quantum Chemistry**, by J. P. Lowe, Academic Press, San Diego, pp 552-553.

APPENDIX 11

BRA–KET NOTATION

Bra–ket, or Dirac, notation is frequently used in the literature because of its economical form. Perhaps the best way to learn how this notation is used is by studying its use in a few familiar relations and proofs. Accordingly, we have outlined a few of these uses. The applications and subtleties of this notation go considerably beyond the treatment summarized here.[1]

"Usual" notation		Dirac notation	
$\int \phi_m^* \phi_n \, d\tau$	$\equiv$	$\underbrace{\langle \phi_m |}_{\text{bra}} \underbrace{\phi_n \rangle}_{\text{ket}} \equiv \langle m \| n \rangle$	(A11-1)
$\int \phi_m^* A \phi_n \, d\tau$	$\equiv$	$\langle \phi_m \| A \| \phi_n \rangle \equiv \langle m \| A \| n \rangle \equiv A_{mn}$	(A11-2)
$\left[\int \phi_m^* \phi_n \, d\tau \right]^* = \int \phi_n^* \phi_m \, d\tau$		$\langle \phi_m \| \phi_n \rangle^* = \langle \phi_n \| \phi_m \rangle$	
	or		(A11-3)
		$\langle m \| n \rangle^* = \langle n \| m \rangle$	

For hermitian operator A:

$$\int \phi_m^* A \phi_n \, d\tau = \int \phi_n (A\phi_m)^* \, d\tau = \left[\int \phi_n^* A \phi_m \, d\tau \right]^* \qquad \langle m|A|n\rangle = \langle n|A|m\rangle^* \qquad \text{(A11-4)}$$

[1] Strictly speaking, for instance, $\langle \phi_m | \phi_n \rangle$ and $\langle m|n \rangle$ are not identical in meaning. The former refers to specific functions, ϕ_m and ϕ_n, which represent state vectors in a specific representation. The latter refers to the state vectors in *any* representation and hence is a more general expression. Distinctions such as this will not be necessary at the level of this text.

Any function ψ can be written as a sum of a complete set of orthonormal functions ϕ:

$$\psi = \sum_m c_m \phi_m \qquad |\psi\rangle = \sum_m c_m |\phi_m\rangle \equiv \sum_m c_m |m\rangle$$

$$\int \phi_n{}^* \psi \, d\tau = \sum_m c_m \int \phi_n{}^* \phi_m \, d\tau = c_n \qquad \langle n|\psi\rangle = \sum_m c_m \langle n|m\rangle = c_n$$

$$c_n = \int \phi_n{}^* \psi \, d\tau \qquad c_n = \langle n|\psi\rangle$$

$$\psi = \sum_m c_m \phi_m = \sum_m \int \phi_m{}^* \psi \, d\tau \phi_m \qquad |\psi\rangle = \sum_m \langle m|\psi\rangle |m\rangle = \sum_m |m\rangle\langle m|\psi\rangle$$

Example of Use Proof that eigenvalues of A (hermitian) are real.

$$A|m\rangle = a_m|m\rangle \tag{A11-5}$$

$$\langle m|A|m\rangle = a_m \underbrace{\langle m|m\rangle}_{\neq 0,\ \neq \infty}, \tag{A11-6}$$

$$\langle m|A|m\rangle^* = a_m{}^* \langle m|m\rangle \tag{A11-7}$$

Combining Eqs. (A11-4), (A11-6), and (A11-7), we have

$$(a_m - a_m{}^*) = 0 \qquad \text{Q.E.D.}$$