## Bra-ket Notation and Linear Algebra

Eigenstate: Bra-ket Vector

Time-independent quantum mechanical states: $|\psi\rangle, \quad \langle\psi|$ (1)

At the beginning, we can understand that the Bra-ket notation simplifies the wavefunctions and their complex conjugate ones. To say more rigorously, the wavefunction $\psi(\boldsymbol{r})$ is a representation of the state $|\psi\rangle$ in coordinate space. The state $\langle\psi|$ is always found along with $|\psi\rangle$ as a pair in dual space. $|\psi\rangle$ is called "ket" vector, and the adjoint of this vector denoted by $\langle\psi|$, we call it "bra" vector. The time-independent Shrodinger's equation for this set of state is:

$$H|\psi\rangle = E|\psi\rangle \tag{2}$$

Then any energy state vector $|\psi\rangle$ can be written as linear superposition of energy eigenstates:

$$|\psi\rangle = \sum_n |\phi_n\rangle c_n, \quad \langle\psi| = \sum_n c_n^* \langle\phi_n| \tag{3}$$

The orthonormality condition can be written:

$$\begin{cases} \int \mathrm{d}^3\boldsymbol{r}\phi_n^*(\boldsymbol{r})\phi_m(\boldsymbol{r}) = \delta_{n,m} \\ \langle\phi_n|\phi_m\rangle = \delta_{n,m} \end{cases} \tag{4}$$

Assuming $|\psi\rangle$ is normalized and that $\langle\psi|\psi\rangle = 1$, we find:

$$\sum_n |c_n|^2 = 1 \tag{5}$$

We can interpret $c_n$ as:

$$c_n = \int \mathrm{d}^3\boldsymbol{r}\phi_n^*(\boldsymbol{r})\psi(\boldsymbol{r}) = \langle\phi_n|\psi\rangle \tag{6}$$

The expectation value of a linear operator $\hat{A}$ in the state $\psi$ is:

$$\bar{A} = \int \mathrm{d}^3\boldsymbol{r}\psi^*(\boldsymbol{r})\hat{A}\psi(\boldsymbol{r})$$

With an application (3):

$$\bar{A} = \sum_{nm} c_n^* c_m A_{nm},$$

$$A_{nm} = \int \mathrm{d}^3\boldsymbol{r}\phi_n^*(\boldsymbol{r})\hat{A}\phi_m(\boldsymbol{r}) \tag{7}$$

With a bracket notation:

$$A_{nm} = \langle \phi_n | \hat{A} | \phi_m \rangle \tag{7'}$$

We can also represent the linear operator $\hat{A}$ with bracket notation:

$$\hat{A} = \sum_{n,m} |\phi_n\rangle A_{nm} \langle \phi_m| \tag{8}$$

Then we can write the coefficients as a column vector:

$$|\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \end{pmatrix} \tag{9a}$$

$$\langle \psi| = (c_0^* c_1^* c_2^* \cdots) \tag{9b}$$

This may be written in matrix notation as:

$$\hat{A} = \begin{pmatrix} A_{00} A_{01} A_{02} \cdots \\ A_{10} A_{11} A_{12} \cdots \\ \cdots\cdots \end{pmatrix} \tag{9c}$$

The operation rule toward the operator bracket vector can be written:

$$\hat{A}|\psi\rangle = \begin{pmatrix} A_{00} A_{01} A_{02} \cdots \\ A_{10} A_{11} A_{12} \cdots \\ \cdots\cdots \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix} \tag{10a}$$

$$\langle \psi|\hat{A} = (c_0^* c_1^* c_2^* \cdots) \begin{pmatrix} A_{00} A_{01} A_{02} \cdots \\ A_{10} A_{11} A_{12} \cdots \\ \cdots\cdots \end{pmatrix} \tag{10b}$$

The inner product of the bracket when we assume $|\phi\rangle = \sum_n d_n |\phi_n\rangle$ is written as:

$$\begin{aligned} \langle \psi|\phi\rangle &= \int \mathrm{d}^3 \boldsymbol{r} \psi^*(\boldsymbol{r})\phi(\boldsymbol{r}) \\ &= (c_0^* c_1^* c_2^* \cdots) \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \end{pmatrix} = \sum_m c_m^* d_m \end{aligned} \tag{10c}$$

(10c) satisfies exactly the same property of the vector inner product:

$$\langle c\psi|\phi\rangle = c^*\langle\psi|\phi\rangle, \qquad \langle\psi|c\phi\rangle = c\langle\psi|\phi\rangle, \tag{11a}$$

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*, \tag{11b}$$

$$\langle\psi|\psi\rangle \geq 0, \tag{11c}$$

$$\langle\psi|\psi\rangle = 0 \longleftrightarrow |\psi\rangle = 0 \tag{11d}$$

Thus we can call $\langle\psi|\phi\rangle$ as "inner product".

The condition for the completeness is frequently written as:

$$\sum_m |\phi_m\rangle\langle\phi_m| = 1 \tag{12}$$

Based on this representation, we can write the projection operator as:

$$P_n = |\phi_n\rangle\langle\phi_n|, \quad P_n|\psi\rangle = |\phi_n\rangle c_n$$

**The Basis Transformation**

The transformation from an old basis $|\phi_n\rangle$ to a new basis $|\chi_n\rangle$ is written as:

$$|\chi_m\rangle = \sum_n |\phi_n\rangle U_{nm}, \qquad U_{nm} = \langle\phi_n|\chi_m\rangle \tag{13}$$

We can obtain a definition of the transformation matrix to be:

$$U = (U_{nm}) \tag{14}$$

An inner product of the new basis then becomes:

$$\langle\chi_{m'}|\chi_m\rangle = \sum_{nn'} U^*_{n'm'} U_{nm} \langle\phi_{n'}|\phi_n\rangle$$

Given the fact that both $\{|\chi_m\rangle\}$ and $\{\phi_m\rangle\}$ are the orthonormality basis then:

$$\sum_n U^*_{nm'} U_{nm} = \delta_{mm'}, \tag{15}$$

Accordingly, we define U as unitary matrix also as unitary transformation.
By calculated inversely (13) can be written:

$$|\phi_n\rangle = \sum_m |\chi_m\rangle (U^{-1})_{mn} = \sum_m |\chi_m\rangle U^*{}_{nm} \tag{13'}$$

We now have:

$$|\psi\rangle = \sum_m |\chi_m\rangle (\sum_n U^*{}_{nm} c_n)$$

We can derive:

$$|\psi\rangle = \sum_m |\chi_m\rangle d_m \tag{16}$$

So, we obtain:

$$d_m = \sum_n U^*{}_{nm} c_n$$
$$c_n = \sum_m U_{nm} d_m \tag{17}$$

Or:

$$(d) = U^\dagger(c), \qquad (c) = U(d)$$

In another way of expression:

$$d_i = \langle \chi_i | \psi \rangle,$$
$$c_n = \langle \phi_n | \psi \rangle,$$
$$U_{ni} = \langle \phi_n | \chi_i \rangle. \tag{17'}$$

$$\langle \chi_i | \psi \rangle = \sum_n U^*{}_{ni} \langle \phi_n | \psi \rangle \tag{17''}$$

Now let's find out a matrix representation of the operator $\hat{A}$.

$$\langle \chi_m | \hat{A} | \chi_{m'} \rangle = \sum_{nn'} U^*{}_{nm} U_{n'm'} \langle \phi_n | \hat{A} | \phi_{n'} \rangle$$
$$= \sum_{nn'} (U^\dagger)_{mn} \langle \phi_n | \hat{A} | \phi_{n'} \rangle U_{n'm'} \tag{18}$$

$$\langle \chi_m | \hat{A} | \chi_n \rangle = A^\chi_{mn} \tag{19}$$

When we define matrix $\hat{A}^\chi$ to be:

$$\hat{A}^\chi = \begin{pmatrix} A^\chi_{00} & A^\chi_{01} & A^\chi_{02} & \cdots \\ A^\chi_{10} & A^\chi_{11} & A^\chi_{12} & \cdots \\ A^\chi_{20} & A^\chi_{21} & A^\chi_{22} & \cdots \\ & & & \cdots \end{pmatrix} \tag{20}$$

Then we can obtain:

$$\hat{A}^\chi = U^\dagger \hat{A}^\phi U \tag{21}$$

This is the transformation of matrix representation according to the transformation of the basis that we are familiar with from studying linear algebra. We can also say that it is a transformational condition for the physical quantity according to the transformation of the basis vectors. The transformation from the Schrodinger's equation to the Heisenberg's equation of motion is represented in the same way.