Lecture 2: Dirac notation and a review of linear algebra

Read Sakurai chapter 1, Baym chatper 3

1 State vector space and the dual space

Space of wavefunctions The space of wavefunctions is the set of all the possible wavefunctions of a given system. $\Psi_1(\xi)$, $\Psi_2(\xi)$, ..., are wavefunctions in the representation of ξ. ξ can be general. For example, in the coordinate representation $\xi = (\vec{q}, \sigma)$, where $\vec{q}$ represents the set of coordinates $(\vec{q}_1, ...\vec{q}_N)$, and σ represents the set of particle spin $(\sigma_{1,z}, ..., \sigma_{2,z})$. The inner product between two wavefunctions are defined as

$$(\Psi_A, \Psi_B) = \int d\xi \Psi^*(\xi)\Psi(\xi) = \sum_{\sigma_{1,z},...,\sigma_{N,z}} \int d\vec{q}_1 ... d\vec{q}_N \Psi^*_{\sigma_1\sigma_2...\sigma_N}(\vec{q}_1, ..\vec{q}_N)\Psi_{\sigma_1\sigma_2...\sigma_N}(\vec{q}_1, .., \vec{q}_N). \quad (1)$$

Space of state vectors (right-vectors); the Hilbert space More conveniently, we use the notation of the state vector $|\Psi\rangle$ (right/ket-vector) to represent a wavefunction $\Psi(\xi)$ of a given quantum system. The advantage of the state vector notation is that it does not depend on concrete representations. All the state vectors $|\Psi\rangle$ span the linear space denoted as the Hilbert space $\mathcal{H}$ of a given quantum system. The following correspondence between a wavefunction and a state vector is defined as:

1) $\Psi(\xi) \longleftrightarrow |\Psi\rangle$;
2) $c_1\Psi_1(\xi) + c_2\Psi_2(\xi) \longleftrightarrow c_1|\Psi_1\rangle + c_2|\Psi_2\rangle$;
3) The inner product: $(\Psi_1, \Psi_2) \longleftrightarrow (|\Psi_1\rangle, |\Psi_2\rangle)$.

The orthonormal complete bases for the space of state vectors For an orthonormal complete bases Ψ_α, we have

$$(\Psi_\alpha, \Psi^{\prime}_\alpha) = \delta(\alpha, \alpha^{\prime}), \qquad \sum_\alpha \Psi_\alpha(\xi)\Psi^*_\alpha(\xi^{\prime}) = \delta(\xi - \xi^{\prime}). \quad (2)$$

For any wavefunction Ψ, we can expand it as

$$\Psi(\xi) = \sum_\alpha \Psi_\alpha(\xi)(\Psi_\alpha(\xi), \Psi), \quad (3)$$

and the inner product as

$$(\Psi^{\prime}, \Psi) = \sum_\alpha (\Psi_\alpha, \Psi^{\prime})^*(\Psi_\alpha, \Psi), \quad (4)$$

Using the formalism of right-vectors, we use $|\Psi_\alpha\rangle$ to represent the wavefunction of

$\Psi_\alpha(\xi)$, and rewrite the above equations as

$$\begin{aligned}(|\Psi_\alpha\rangle, |\Psi_{\alpha}^{\prime}\rangle &= \delta(\alpha,\alpha^{\prime}), \quad |\Psi\rangle = \sum_\alpha |\Psi_\alpha\rangle(|\Psi_\alpha\rangle, |\Psi\rangle), \\ (|\Psi^{\prime}\rangle, |\Psi\rangle) &= \sum_\alpha (|\Psi_\alpha,\rangle|\Psi^{\prime}\rangle)^*(|\Psi_\alpha\rangle, |\Psi\rangle),\end{aligned} \tag{5}$$

where $(|\Psi_\alpha\rangle, |\Psi\rangle)$ is the coordinate of the state vector $|\Psi\rangle$ projection to the basis $|\Psi_\alpha\rangle$.

The dual space (space of left-vectors) The right-vector space $\mathcal{H}$ is a linear space. All the linear mappings from the right-vector space $\mathcal{H}$ to the complex number field C also form a linear space, which is denoted as the dual space. We use left-vector (bra-vector) to denote an element in the dual space. Let us consider a linear mapping denoted by $\langle A|$ in the dual space, which can be determined by its operation on the orthonormal bases Φ_α in the Hilbert space $\mathcal{H}$.

$$\langle A : |\Phi_\alpha\rangle \to a_\alpha^*, \tag{6}$$

where a_α^* is a complex number, and α is the index to mark the orthonormal bases. Then for any right-vector $|B\rangle = \sum_\alpha b_\alpha |\Psi_\alpha\rangle$ where $b_\alpha = (|B\rangle, |\Psi_\alpha\rangle)$, the operation of $\langle A|$ on $|B\rangle$ is represented as

$$\langle A| : |B\rangle \to \sum_\alpha a_\alpha^* b_\alpha. \tag{7}$$

We can identify a one-to-one correspondence between a right-vector and a linear mapping (a left-vector) as

$$\langle A| \longleftrightarrow |A\rangle = a_\alpha |\Phi_\alpha\rangle, \tag{8}$$

such that the operation of $\langle A|$ on any right-vector $|B\rangle$ is expressed as

$$\langle A| : |B\rangle \to \sum_\alpha a_\alpha^* b_\alpha = (|A\rangle, |B\rangle). \tag{9}$$

Below we will simply use the notation $\langle A|B\rangle$ to denote the mapping $\langle A| : |B\rangle$. Using these notations, we can rewrite Eq. 5 as

$$\langle \Psi_\alpha|\Psi_{\alpha}^{\prime}\rangle = \delta(\alpha,\alpha^{\prime}), \qquad |\Psi\rangle = \sum_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|\Psi\rangle. \tag{10}$$

We define the conjugation operation for left and right vectors, and complex numbers as

$$\overline{|\Psi\rangle} = \langle\Psi|; \quad \overline{\langle\phi|} = |\phi\rangle; \quad \bar{a} = a^*, \tag{11}$$

thus we have

$$\overline{a|A\rangle} = \langle A|\bar{a}, \quad \overline{a\langle B|} = |B\rangle\bar{a}. \tag{12}$$

2 Operator of an observable

We define the linear operator L acting on the right-vectors in $\mathcal{H}$, which satisfies

1) $L|B\rangle$ is still a right-vector in $\mathcal{H}$,
2) $L(b|B\rangle + c|C\rangle) = bL|B\rangle + cL|C\rangle$.
L can be determined through its operation on the orthonormal basis $|\Phi_\beta\rangle$ of $\mathcal{H}$ as

$$L|\Phi_\beta\rangle = \sum_\alpha L_{\alpha\beta}|\Phi_\alpha\rangle, \tag{13}$$

where $L_{\alpha\beta} = \langle\Psi_\alpha|L|\Psi_\beta\rangle$ is the matrix element of L for the basis of Φ_α.

For any state-vector $|B\rangle = \sum_\alpha b_\alpha|\Phi_\alpha\rangle$, the operation of L is

$$L|B\rangle = \sum_\beta b_\beta L|\Phi_\beta\rangle = \sum_{\alpha\beta} L_{\alpha\beta} b_\beta |\Phi_\alpha\rangle. \tag{14}$$

The operation of L on the left vectors can also be defined. For a given $\langle A|$, the operation of $\langle A|L$ is defined through the following equation

$$\langle A|L : |B\rangle = \langle A|L|B\rangle, \tag{15}$$

where $|B\rangle$ is an arbitrary right-vector. Thus $\langle A|L$ is a linear mapping from the right-vector space to complex numbers, thus it should be represented by a left-vector $\langle\phi| = \langle A|L$, such that $\langle A|L : |B\rangle = \langle\phi|B\rangle$.

The conjugation operations We further extend the definition of conjugation operation below

$$\begin{aligned} \langle\Psi_1|\overline{L}|\Psi_2\rangle &= \overline{\langle\Psi_2|L|\Psi_1\rangle}, \\ \overline{L_1 L_2} &= \overline{L_2}\ \overline{L_1}, \\ \overline{L|\Psi\rangle} &= \langle\Psi|\overline{L}, \\ \overline{\langle A|B\rangle} &= \langle B|A\rangle. \end{aligned} \tag{16}$$

In the following, we denote $\overline{L}$ as $L^\dagger$.

In the orthonormal basis Ψ_α, the matrix elements of $L^\dagger$ reads

$$L^\dagger_{\alpha\beta} = \langle\Psi_\alpha|L^\dagger|\Psi_\beta\rangle = \overline{\langle\Psi_\beta|L|\Psi_\alpha\rangle} = L^*_{\beta\alpha}. \tag{17}$$

If the operators $L = L^\dagger$, i.e., $L_{\alpha\beta} = L^*_{\beta\alpha}$, we call that L is *Hermitian*.

3 Outer product between left and right-vectors as operators

We define $|A\rangle\langle B|$ as a linear operator. When acting on a right-vector $|\Psi\rangle$, it behaves as

$$(|A\rangle\langle B|)|\Psi\rangle = |A\rangle\langle B|\Psi\rangle. \tag{18}$$

Corollary:

1)$\langle\Psi|(|A\rangle\langle B|) = \langle\Psi|A\rangle\langle B|$,

2) $\overline{|A\rangle\langle B|} = |B\rangle\langle A|$,

3) $|A\rangle\langle A|$ is Hermitian.

4) $\overline{|A\rangle\langle B|\Psi\rangle} = \langle\Psi|B\rangle\langle A| = \overline{|\Psi\rangle} \quad \overline{|A\rangle\langle B|}$.

5) For a set of orthonormal bases $|\Psi_\alpha\rangle$, from Eq. 5, we have

$$I = \sum_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|, \tag{19}$$

where I is the identity operator.

6) Expansion of a linear operator L as

$$L = \sum_{\alpha\alpha^{'}} |\Psi_\alpha\rangle\langle\Psi_\alpha|L|\Psi_{\alpha^{'}}\rangle\langle\Psi_{\alpha^{'}}| = \sum_{\alpha\alpha^{'}} |\Psi_\alpha\rangle\langle\Psi_{\alpha^{'}}|L_{\alpha\alpha^{'}}, \tag{20}$$

where $L_{\alpha\alpha^{'}} = \langle\Psi_\alpha|L|\Psi_{\alpha^{'}}\rangle$ is the matrix element under the bases of $|\Psi_\alpha\rangle$.

Examples:

1)For a single spinless particle, we denote $|\vec{r}\rangle$ as the eigenstate of the coordinate operator $\vec{r}$, which satisfy the orthonormal condition $\langle\vec{r}|\vec{r}^{'}\rangle = \delta(\vec{r}-\vec{r}^{'})$. We have

$$\int d\vec{r}|\vec{r}\rangle\langle\vec{r}| = I, \tag{21}$$

thus

$$\int d\vec{r}|\vec{r}\rangle\langle\vec{r}|\Psi\rangle = |\Psi\rangle, \tag{22}$$

and

$$\int d\vec{r}^{'}\langle\vec{r}|\vec{r}^{'}\rangle\langle\vec{r}^{'}|\Psi\rangle = \langle\vec{r}|\Psi\rangle = \Psi(\vec{r}). \tag{23}$$

Similarly, for an orthonormal basis Ψ_α, we have

$$\begin{aligned}\sum_\alpha \Psi^*_\alpha(\vec{r})\Psi_\alpha(\vec{r}^{\,\prime}) &= \sum_\alpha \langle\vec{r}|\Psi_\alpha\rangle^*\langle\vec{r}^{\,\prime}|\Psi_\alpha\rangle = \sum_\alpha \langle\vec{r}^{\,\prime}|\Psi_\alpha\rangle\langle\Psi_\alpha|\vec{r}\rangle = \langle\vec{r}^{\,\prime}|\{\sum_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha\}|\vec{r}\rangle \\ &= \langle\vec{r}^{\,\prime}|\vec{r}\rangle = \delta(\vec{r}-\vec{r}^{\,\prime}). \end{aligned} \tag{24}$$

4 Representations and transformation of representations

When we fix a set of orthonormal bases $|\Psi_\alpha\rangle$ for the Hilbert space, it means that we are using a specific representation. We can express a state vector $|\Psi\rangle$ and a linear operator L as matrices as

$$\begin{aligned}|A\rangle &= \sum_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|A\rangle, \\ L &= \sum_{\alpha\alpha'} |\Psi_\alpha\rangle\langle\Psi'_\alpha|\langle\Psi_\alpha|L|\Psi'_\alpha\rangle, \end{aligned} \tag{25}$$

and

$$\begin{aligned}\langle A|B\rangle &= \sum_\alpha \langle A|\Psi_\alpha\rangle\langle\Psi_\alpha|B\rangle \\ \langle A|L|B\rangle &= \sum_{\alpha'} \langle\Psi_\alpha|A\rangle^* L_{\alpha\beta}\langle\Psi_\alpha|B\rangle. \end{aligned} \tag{26}$$

Using the matrix notation, we denote $A_\alpha = \langle\Psi_\alpha|A\rangle$, then in the representation of $|\Psi_\alpha\rangle$, $|A\rangle$ is represented by a column vector of A_α, and L is represented by a matrix $L_{\alpha\beta}$. In the matrix notation, we have

$$\langle A|B\rangle = \sum_\alpha A^*_\alpha B_\alpha, \quad \langle A|L|B\rangle = \sum_{\alpha\beta} A^*_\alpha L_{\alpha\beta} B_\beta. \tag{27}$$

Let us choose another set of orthonormal basis $|\varphi_\lambda\rangle$, which satisfy $\sum_\lambda |\varphi_\lambda\rangle\langle\varphi_\lambda| = I$. The transformation matrix U between these two sets of bases is defined as

$$|\varphi_\lambda\rangle = \sum_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|\varphi_\lambda\rangle = \sum_\alpha |\Psi_\alpha\rangle U_{\alpha\lambda}, \tag{28}$$

where $U_{\alpha\lambda} = \langle\Psi_\alpha|\varphi_\lambda\rangle$. U is an unitary matrix, which satisfies the following relation

$$U^\dagger U = UU^\dagger = I. \tag{29}$$

For an arbitrary state vector $|A\rangle$, its coordinate $\langle\Psi_\alpha|A\rangle$ in the $|\Psi\rangle$ representation can be expressed in terms of its coordinates in the $|\varphi\rangle$ representation through the transformation matrix

U as

$$\langle\Psi_\alpha|A\rangle = \sum_\lambda \langle\Psi_\alpha|\varphi_\lambda\rangle\langle\varphi_\lambda|A\rangle = \sum_\lambda U_{\alpha\lambda}\langle\varphi_\lambda|A\rangle. \tag{30}$$

And for the matrix element $L_{\alpha\alpha'}$ in the $|\Psi\rangle$-representation can also be related to that in the in the $|\varphi\rangle$ representation as

$$\langle\Psi_\alpha|L|\Psi_{\alpha'}\rangle = \sum_{\lambda\lambda'} \langle\Psi_\alpha|\varphi_\lambda\rangle\langle\varphi_\lambda|L|\varphi_{\lambda'}\rangle\langle\varphi_{\lambda'}|\Psi_{\alpha'}\rangle = U_{\alpha\lambda}\langle\varphi_\lambda|L|\varphi_{\lambda'}\rangle U^\dagger_{\lambda\alpha'}. \tag{31}$$