Lecture 14
Formal
development on
symmetries

Equations of motion and canonical quantization

Read Sakurai Chapter 1.6 and 1.7

In Lecture 1 and 2, we have discussed how to represent the state of a quantum mechanical system based the superposition principle and statistical interpretation. Now we need to solve the problem of the time evolution of quantum mechanical states.

1 Equation of motion: the Schrödinger equation

Time-evolution operator We start with the time evolution of a pure state. Suppose that at time t_0, the state is $|\Psi(t_0)\rangle$. Let it evolve to time t, the state becomes $|\Psi(t)\rangle$. We define the time evolution operator $T(t,t_0)$ which is determined by the system, say, the mass of particles and interactions among them. But $T(t,t_0)$ does not depend on which state it applies. Before we derive the concrete form of $T(t,t_0)$, we should be able to conclude that it satisfies the following properties.

1. $T(t,t_0)$ should be a linear operator as required by the superposition principle, *i.e.*,

$$T(t,t_0)(c_1|\Psi_1(t_0)\rangle + c_2|\Psi_2(t_0)\rangle) = c_1 T(t,t_0)|\Psi_1(t_0)\rangle + c_2 T(t,t_0)|\Psi_2(t_0)\rangle. \tag{1}$$

2. $T(t_0,t_0) = 1$.

3. $T(t_2,t_0) = T(t_2,t_1)T(t_1,t_0) = 1$.

4. $T(t_0,t_1)T(t_1,t_0) = T(t_1,t_0)T(t_0,t_1) = 1$, or $T^{-1}(t_0,t_1) = T(t_1,t_0)$.

5. Once $|\Psi(t_0)\rangle$ is normalized, *i.e.*, $\langle\Psi(t_0)|\Psi(t_0)\rangle = 1$, then at time t, $|\Psi(t)\rangle$ should also be normalized, *i.e.*, $\langle\Psi(t)|\Psi(t)\rangle = 1$. Thus T should be a unitary operator $T^\dagger(t_1,t_0)T(t_1,t_0) = 1$. From 4. and 5, we have

$$T^\dagger(t,t_0) = T(t_0,t). \tag{2}$$

6. For two independent systems A and B, the state vectors can be written as a tensor product $|\phi_A(t)\rangle \otimes |\phi_B(t)\rangle$, the total time evolution operator $T_{AB}(t_1,t_0) = T_A(t_1,t_0) \otimes T_B(t_1,t_0)$.

Equations of motion We can write down equations of motion of state vectors based on the infinitesimal generator of T. Let us take the first order time derivative of $|\Psi(t)\rangle$ as

$$\frac{\partial\Psi(t)}{\partial t} = \lim_{t' \to t} \frac{\Psi(t') - \Psi(t)}{t' - t} = \lim_{t' \to t} \frac{T(t',t) - 1}{t' - t}\Psi(t) = \frac{\partial T(t',t)}{\partial t'}\Big|_{t'=t}\Psi(t). \tag{3}$$

Next we prove that $\frac{\partial T(t^{'},t)}{\partial t^{'}}|_{t^{'}=t}$ is an anti-Hermitian operator. From $T^{\dagger}(t^{'},t)T(t^{'},t)=1$, we have

$$\frac{\partial T^{\dagger}(t^{'},t)}{\partial t^{'}}T(t^{'},t)+T^{\dagger}(t^{'},t)\frac{\partial T(t^{'},t)}{\partial t^{'}}=0. \tag{4}$$

Set $t^{'}\to t$, we have

$$\frac{\partial T^{\dagger}(t^{'},t)}{\partial t^{'}}|_{t^{'}=t}+\frac{\partial T(t^{'},t)}{\partial t^{'}}|_{t^{'}=t}=0. \tag{5}$$

We set $\hat{M}(t)\equiv i\partial T(t^{'},t)/\partial t^{'}|_{t^{'}=t}$, then $\hat{M}(t)$ is a Hermitian operator and

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle=\hat{M}(t)|\Psi(t)\rangle. \tag{6}$$

$\hat{M}(t)$ should be a linear operator as required by superposition principle, and its Hermiticity comes from the unitarity of time evolution operator. $\hat{M}(t)$ is also additive, i.e. for two independent systems A and B, we should have $\hat{M}_{AB}(t)=\hat{M}_A(t)+\hat{M}_B(t)$.

Then what is $\hat{M}$?

Why Hamiltonian? Consider an infinitesimal time interval Δt, and expand $|\Psi(t-\Delta t\rangle=|\Psi(t)\rangle+i\Delta t\hat{M}(t)|\Psi(t)\rangle$, then

$$\langle\Psi(t-\Delta t)|\Psi(t)\rangle-\langle\Psi(t)|\Psi(t)\rangle\sim i\Delta t\langle\Psi(t)|\hat{M}(t)|\Psi(t)\rangle. \tag{7}$$

Consider a time-translation invariant system, and take the limit $\Delta t\to 0$, we have

$$\lim_{\Delta t\to 0}\frac{\langle\Psi(t-\Delta t)|\Psi(t)\rangle-\langle\Psi(t)|\Psi(t)\rangle}{\Delta t}=\langle\Psi(t)|i\hat{M}(t)|\Psi(t)\rangle. \tag{8}$$

The left-hand-side is independent of t because time-translation symmetry, thus $\langle\Psi(t)|i\hat{M}(t)|\Psi(t)\rangle$ should be a conserved quantity. Such a conserved quantity originates from the time translation symmetry, and it is also additive. In classic theory, it is nothing but Hamiltonian up to a constant, and we denote this constant as $\hbar$, i.e., $\hbar\hat{M}=\hat{H}$. Now we have the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle=\hat{H}|\Psi(t)\rangle. \tag{9}$$

2 Canonical quantization

Still, we need to determine the operator of Hamiltonian. Actually, every quantum theory originates from a classic theory. The process from classic theory to quantum theory is called quantization. A common method is the so-called canonical quantization with the following steps. The process of canonical quantization ensures that quantum mechanical equations of motions have a classic correspondence.

1. (Classic mechanics) Determine the classic Hamiltonian and classic mechanical observables as functions of a set of fundamental observables. Usually, the fundamental observables are chosen as canonical coordinates and momenta.

2. (Canonical quantization condition) Determine the operators of the fundamental observables. The relation between operators of canonical coordinates and momenta are called quantization condition.

3. (QM) Assume the relations between operators of observables and the fundamental operators in quantum mechanics are the same as those in classical mechanics by the spirit of the correspondence principle.

3 Operators of momenta of the Cartesian coordinates

We have derived before that the operator of coordinate in the coordinate representation is just the coordinate itself. Now we need to derive the operator for momentum.

We start from the translation operator $U(\vec{R})$ under the spatial translation $\vec{R}$. In classic mechanics, the coordinate and momentum transform as

$$(\vec{r},\vec{p}) \longrightarrow (\vec{r}+\vec{R},\vec{p}). \tag{10}$$

In quantum mechanics, for a state vector $|\Psi\rangle$, we denote that after such a translation,

$$|\Psi^R\rangle = U(\vec{R})|\Psi\rangle. \tag{11}$$

For two successive translations $\vec{R}_1$ and $\vec{R}_2$, their total effect is equivalent to a new translation $\vec{R}_3 = \vec{R}_1 + \vec{R}_2$. At current stage, we only consider the case without magnetic field, such that any two translations commute. We require that U satisfies

$$U(\vec{R}_3) = U(\vec{R}_1)U(\vec{R}_2). \tag{12}$$

In a later lecture of space-time symmetry, we can prove that U should be a unitary linear operator. Now, we assume it is true. We require the following properties for $U(\vec{R})$:

1. $U(0) = 1$.

2. $\langle\Psi^R| = \langle\Psi|U^\dagger(\vec{R})$

3. $\langle\Psi^R|\Psi^R\rangle = \langle\Psi|\Psi\rangle, \longrightarrow U^\dagger(\vec{R})U(\vec{R}) = 1$.

4. $\langle\Psi^R|\hat{\vec{r}}|\Psi^R\rangle = \langle\Psi|\hat{\vec{r}}+\vec{R}|\Psi\rangle \longrightarrow U^\dagger(\vec{\delta})\hat{\vec{r}}U(\vec{\delta}) = \hat{\vec{r}}+\vec{R}$.

5. $\langle\Psi^R|\hat{\vec{P}}|\Psi^R\rangle = \langle\Psi|\hat{\vec{P}}|\Psi\rangle \longrightarrow U^\dagger(\vec{R})\hat{\vec{P}}U(\vec{R}) = \hat{\vec{P}}$.
6. $\langle\Psi^R|\hat{\vec{S}}\Psi^R\rangle = \langle\Psi|\hat{\vec{S}}|\Psi\rangle \longrightarrow U^\dagger(\vec{R})\hat{\vec{S}}U(\vec{R}) = \hat{\vec{S}}$.
7. For two subsystems $|\psi_A\rangle$ and $|\psi_B\rangle$, we have $U_{AB}(\vec{R})[|\psi_A\rangle\otimes|\psi_B\rangle] = [U_A(\vec{R})|\psi_A\rangle]\otimes[U_B(\vec{R})|\psi_B\rangle]$.
8. We also fix the convention of the phase of U. For coordinate eigenstate $|\vec{r}^{\,\prime}\rangle$, whose wavefunction in the coordinate representation is $\delta(\vec{r}-\vec{r}^{\,\prime})$, $U|\vec{r}^{\,\prime}\rangle = |\vec{r}^{\,\prime}+\vec{R}\rangle$.

Consider an infinitesimal translation with $\vec{\delta}\sim 0$, and thus $U(\vec{\delta}) = 1+\vec{\delta}\cdot\frac{\partial U(\vec{\delta})}{\partial\vec{\delta}}$, we have

$$\langle\Psi(t)|U(\vec{\delta})|\Psi(t)\rangle \approx \langle\Psi(t)|\Psi(t)\rangle + \vec{\delta}\cdot\langle\Psi(t)|\frac{\partial U(\vec{\delta})}{\partial\vec{\delta}}|\Psi(t)\rangle. \tag{13}$$

If the space is translationally invariant, which means that if $|\Psi(t)\rangle$ represents a possible time-dependent state of the system, so does $|\Psi^{\prime}(t)\rangle = U(\delta)|\Psi(t)\rangle$. We also assume the time translation symmetry of the system, then $\langle\Psi(t)|\Psi^{\prime}(t)\rangle$ should be independent of t. Thus, $\langle\Psi|\frac{\partial U(\vec{\delta})}{\partial\vec{\delta}}|\Psi\rangle$ is a conserved quantity associated with space translation symmetry. Furthermore, for two subsystems with states $|\psi_A\rangle$ and $|\psi_B\rangle$, $\frac{\partial U(\vec{\delta})}{\partial\vec{\delta}}$ is additive, *i.e.*,

$$\langle\psi_{AB}|\frac{\partial U_{AB}(\vec{\delta})}{\partial\vec{\delta}}|\Psi_{AB}\rangle = \langle\psi_A|\frac{\partial U_A(\vec{\delta})}{\partial\vec{\delta}}|\Psi_A\rangle + \langle\psi_B|\frac{\partial U_B(\vec{\delta})}{\partial\vec{\delta}}|\Psi_B\rangle. \tag{14}$$

From above properties, $\frac{\partial U(\vec{\delta})}{\partial\vec{\delta}}$ should be proportional to the total momentum up to a constant

$$\hat{\vec{P}} = iC\frac{\partial U(\vec{\delta})}{\partial\vec{\delta}}|_{\delta=0}. \tag{15}$$

P is a Hermitian operator. Later, we will prove that C is actually just $\hbar$. Let us use it now.

For simplicity, let us consider one-dimensional translation and drive its operator for finite distance translation R. From Eq. 15, we have

$$U(R+\delta) = U(R)U(\delta) \approx U(R)(1-\frac{i}{\hbar}p\delta) \tag{16}$$

and thus

$$\frac{\partial}{\partial_R}U(\vec{R}) = -\frac{ip}{\hbar}U(\vec{R}), \tag{17}$$

and thus

$$U(R) = e^{-\frac{i}{\hbar}pR}. \tag{18}$$

For the 3-dimensional translation, we can generalize the above result as

$$U(\vec{R}) = \exp\{-\frac{i}{\hbar}\vec{R}\cdot\vec{P}\}, \tag{19}$$

where $\vec{R}$ is a 3-vector.

Now let us consider the coordinate eigenstate $|\vec{r}\rangle$. The effect of an infinitesimal translation along the x-direction is

$$U(\delta\hat{e}_x)|\vec{r}\rangle = |\vec{r}+\delta\hat{e}_x\rangle \approx (1-\frac{i}{\hbar}\hat{P}_x\delta)|\vec{r}\rangle. \tag{20}$$

Then we have

$$\hat{P}_x|\vec{r}\rangle \quad = \quad \imath\hbar\vec{\nabla}_x|\vec{r}\rangle. \tag{21}$$

Please note that $\vec{\nabla}_{r_i}$ here is not an operator, it is just a derivative with respect to eigenvalues of $\vec{r}_1$, i.e.,

$$\nabla_x|\vec{r}\rangle = \lim_{\delta\to 0}\frac{|\vec{r}+\delta\hat{e}_x\rangle - |\vec{r}\rangle}{\delta}. \tag{22}$$

Then we have

$$\langle\vec{r}|\hat{P}_x|\Psi\rangle = \overline{\langle\Psi|\hat{P}_x|\vec{r}\rangle} = -i\hbar\nabla_x\langle\vec{r}|\Psi\rangle. \tag{23}$$

In terms of wavefunctions, we have

$$(\hat{P}_x\Psi)(\vec{r}) = -i\hbar\nabla_x\Psi(\vec{r}), \tag{24}$$

or, more generally,

$$(\hat{P}_i\Psi)(\vec{r}) = -i\hbar\nabla_i\Psi(\vec{r}). \tag{25}$$

We also have the expression for coordinates before

$$(x_i\Psi)(\vec{r}) = x_i\Psi(\vec{r}). \tag{26}$$

So far, we have both expressions of $\vec{x}$ and $\vec{P}$ in the coordinate representation.

4 Canonical quantization condition

For simplicity, let us consider a single particle, and we have

$$U^\dagger(\vec{\delta})\hat{r}U(\vec{\delta}) = \hat{r}+\vec{\delta}, \quad U^\dagger(\vec{\delta})\hat{p}U(\vec{\delta}) = \hat{p}, \quad U = \exp\{-\frac{i}{\hbar}\vec{\delta}\cdot\vec{P}\}. \tag{27}$$

From $U(\delta_x e_x)\hat{r}U(\delta_x e_x) = \hat{r}+\delta_x$, or,

$$U^\dagger(\delta_x e_x)\hat{x}U(\delta_x e_x) = \hat{x}+\delta_x, \tag{28}$$
$$U^\dagger(\delta_x e_x)\hat{y}U(\delta_x e_x) = \hat{y}, \tag{29}$$
$$U^\dagger(\delta_x e_x)\hat{z}U(\delta_x e_x) = \hat{z}. \tag{30}$$

Taking the limit of $\delta_x \to 0$, we have

$$[\hat{x},\hat{p}_x] = i\hbar, \quad [\hat{x},\hat{p}_y] = 0, \quad [\hat{x},\hat{p}_z] = 0. \tag{31}$$

In general, we have

$$\hat{x}_i^\dagger = \hat{x}_i, \quad \hat{p}_i^\dagger = \hat{p}_i, \quad [\hat{x}_i,\hat{p}_j] = i\hbar\delta_{ij}. \tag{32}$$

This is the quantization condition in the Schödinger picture.

5 Momentum operators in many-particle systems

Now consider a many-particle system, their coordinate eigenstates $|\vec{r}_1,\vec{r}_2,....\rangle$. The effect of the translation operator is

$$U(\vec{R})|\vec{r}_1,\vec{r}_2,....\rangle = |\vec{r}_1+\vec{R},\vec{r}_2+\vec{R},....\rangle. \tag{33}$$

and

$$U(\vec{R}) = e^{-\frac{i}{\hbar}\vec{R}\cdot\vec{P}_{tot}} \tag{34}$$

where $\vec{P}_{tot}$ is the total angular momentum defined as

$$\vec{P}_{tot} = \sum_i \vec{P}_i. \tag{35}$$

The we have

$$\vec{P}_{tot}|\vec{r}_1,\vec{r}_2,....\rangle = \imath\hbar\sum_{r_i}\vec{\nabla}_{r_i}|\vec{r}_1,\vec{r}_2,....\rangle. \tag{36}$$

Again we have

$$\langle\vec{r}_1,\vec{r}_2,...|\hat{P}_{tot}|\Psi\rangle = \overline{\langle\Psi|\hat{P}_{tot}|\vec{r}_1,\vec{r}_2,...\rangle} = -i\hbar\sum_i\nabla_i\langle\vec{r}_1,\vec{r}_2,...|\Psi\rangle. \tag{37}$$

From the additivity of momentum, the momentum for the j-th particle should be

$$\langle\vec{r}_1,\vec{r}_2,...|\vec{p}_j|\Psi\rangle = -i\hbar\vec{\nabla}_j\langle\vec{r}_1,\vec{r}_2,...|\Psi\rangle, \tag{38}$$

, or, in terms of wavefunctions, we have

$$(\hat{p}_j\Psi)(\vec{r}_1,\vec{r}_2,..) = -i\hbar\vec{\nabla}_j\Psi(\vec{r}_1,\vec{r}_2,..). \tag{39}$$

6 Proof of $C = \hbar$

Recall that in Eq. 15, we set the value of $C = \hbar$. Now let us do actually prove it, and thus the canonical quantization condition does not bring a new constant other than $\hbar$. Consider a classic Hamiltonian $H(x,p)$, and we replace x and p with quantum mechanical operators $\hat{x}$ and $\hat{p}$ and then arrive at quantum mechanical Hamiltonian $\hat{H}(\hat{x},\hat{p})$. Consider that in the case that $\hat{H}(\hat{x},\hat{p})$ can be expanded as series of $\hat{x}$ and $\hat{p}$,

$$\hat{H}(\hat{x},\hat{p}) = \sum_{n=1}^{+\infty} a_n\hat{p}^n + \sum_{m=1}^{+\infty} b_m\hat{x}^m. \tag{40}$$

We have

$$[\hat{x},\hat{H}(\hat{x},\hat{p})] = iC\frac{\partial\hat{H}(\hat{x},\hat{p})}{\partial p}, \quad [\hat{p},\hat{H}(\hat{x},\hat{p})] = -iC\frac{\partial\hat{H}(\hat{x},\hat{p})}{\partial x}. \tag{41}$$

Exercise Please prove Eq. 41.

Then from Schrödinger equation $i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$, we have

$$\begin{aligned}
\frac{d}{dt}\langle\Psi(t)|\hat{x}_j|\Psi(t)\rangle &= \frac{i}{i\hbar}\langle\Psi(t)|[\hat{x}_j,H]|\Psi(t)\rangle = \frac{C}{\hbar}\langle\Psi|\frac{\partial\hat{H}}{\partial p}|\Psi\rangle, \\
\frac{d}{dt}\langle\Psi(t)|\hat{p}_j|\Psi(t)\rangle &= \frac{i}{i\hbar}\langle\Psi(t)|[\hat{p}_j,H]|\Psi(t)\rangle = -\frac{C}{\hbar}\langle\Psi|\frac{\partial\hat{H}}{\partial x}|\Psi\rangle.
\end{aligned} \tag{42}$$

Compared to the classic Hamilton equations, we conclude that $C = \hbar$. Thus Schrödinger equation plus quantization condition give rise to a harmonic correspondence between quantum and classic mechanics.

7 Momentum eigenstates and momentum representation

Consider a single particle momentum eigenstate $\hat{p}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle$. In the coordinate representation, we have

$$\langle\vec{r}|\hat{p}|\vec{p}\rangle = \vec{p}\langle\vec{r}|\vec{p}\rangle, \tag{43}$$

or,

$$-i\hbar\nabla\psi_{\vec{p}}(\vec{r}) = \vec{p}\psi_{\vec{p}}(\vec{r}), \tag{44}$$

and thus we have

$$\psi_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}. \tag{45}$$

Eq. 45 is normalized according to

$$\int d^3 r \psi^*_{\vec{p}}(\vec{r}) \psi_{\vec{p}}(\vec{r}) = \delta(\vec{k} - \vec{k}^{\prime}), \tag{46}$$

where $\vec{k} = \vec{p}/\hbar$ is the wavevector. If we consider a finite volume, say, a cubic box with edge length L, the values of k_i are discrete, we use the box renormalization

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{L^{\frac{3}{2}}} e^{i\vec{k}\cdot\vec{r}}, \quad \int d^3 r \psi^*_{\vec{k}}(\vec{r}) \psi_{\vec{k}}(\vec{r}) = \delta_{\vec{k},\vec{k}^{\prime}}. \tag{47}$$

Just like that all the eigenstates of $\hat{x}$ form a complete basis of a single particle Hilbert space, so do the eigenstates of $\hat{p}$. Similar results apply to many-particle systems. Let us denote $|p_1 p_2 ....\rangle$ as the eigenbases of a set of momenta operator $\hat{p}_1, \hat{p}_2, ...$ They satisfy

$$\begin{aligned} \hat{p}_j |p_1 p_2 ...\rangle &= p_j |p_1 p_2 ...\rangle \\ \langle p_1 p_2 ... | p_1^{\prime} p_2^{\prime} ...\rangle &= \delta(p_1 - p_1^{\prime}) \delta(p_2 - p_2^{\prime}) ... \\ \int dp_1 dp_2 ... |p_1 p_2 ..\rangle \langle p_1 p_2 ..| &= I. \end{aligned} \tag{48}$$

For simplicity, let us come back to the single particle cases, and ask what are the expressions of wavefunctions, $\hat{x}$, and $\hat{p}$ in the momentum representation? The wavefunction of the state vector $|\Psi\rangle$ in momentum representation is

$$\Psi(\vec{p}) = \langle \vec{p} | \Psi \rangle. \tag{49}$$

And notice that $\hat{x}|x\rangle = x|x\rangle$, and $\langle p|\hat{p} = p\langle p|$, we have

$$\begin{aligned} \langle p|\hat{x}|\Psi\rangle &= \int dx \langle p|\hat{x}|x\rangle\langle x|\Psi\rangle = \int dx x \langle p|x\rangle\langle x|\Psi\rangle = \int dx x e^{-i\frac{px}{\hbar}} \langle x|\Psi\rangle, \\ &= i\hbar\nabla_p \int dx \langle p|x\rangle\langle x|\Psi\rangle = i\hbar\nabla_p \Psi(p), \end{aligned} \tag{50}$$

$$\langle p|\hat{p}|\Psi\rangle = p\Psi(p). \tag{51}$$

The above equations mean that in the momentum representation

$$\hat{x} = i\hbar\nabla_p, \quad \hat{p} = p. \tag{52}$$

8 Some subtle points

From Eq. 50, we have

$$\langle p|x|\Psi\rangle = i\hbar \lim_{\delta p \to 0} \frac{\langle p+\delta p|\Psi\rangle - \langle p|\Psi\rangle}{\delta p}, \tag{53}$$

thus

$$\langle p|x = i\hbar \nabla_p \langle p|, \tag{54}$$

or

$$x|p\rangle = -i\hbar \nabla_p |p\rangle. \tag{55}$$

Compare the expression proved before

$$p|x\rangle = i\hbar \nabla_x |x\rangle. \tag{56}$$

Lecture 5: Orbital angular momentum, spin and rotation

1 Orbital angular momentum operator

According to the classic expression of orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$, we define the quantum operator

$$L_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, L_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, L_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x. \tag{1}$$

(From now on, we may omit the hat on the operators.) We can check that the three components of operators of $\vec{L}$ are Hermitian, and satisfy the commutation relation

$$[L_i, L_j] = i\varepsilon_{ijk}\hbar L_k. \tag{2}$$

The non-commutativity of $L_i (i = x, y, z)$ is absent in the classic physics, which is a quantum effect. We can normalize L_i by dividing l, roughly speaking the magnitude of orbital angular momentum, we have

$$[\frac{L_i}{l}, \frac{L_j}{l}] = \frac{1}{l} i\varepsilon_{ijk}\frac{L_k}{l}. \tag{3}$$

As we can see, that in the limit of $l \to \infty$, the non-commutativity approaches zero and thus the classic physics is recovered.

2 Rotation operator

Let us define the rotation operator. Consider a single particle state $|\Psi\rangle$, and after a rotation operation $g(\hat{n}, \theta)$ where $\hat{n}$ is the rotation axis and θ is the rotation angle, we arrive at $|\Psi^g\rangle$. The operation of g on three-vectors, such as $\vec{r}$, $\vec{p}$, and $\vec{S}$, is described by a 3×3 special orthogonal matrix, i.e., SO(3), $g_{\alpha\beta}$ as

$$(g\vec{r})_\alpha = g_{\alpha\beta} r_\beta; \quad (g\vec{p})_\alpha = g_{\alpha\beta} p_\beta; \quad (g\vec{S})_\alpha = g_{\alpha\beta} S_\beta. \tag{4}$$

For example, for $\hat{n} = \hat{z}$, we have

$$g(\hat{z}, \theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

For infinitesimal rotation angle θ,

$$g(\hat{z}, \theta) \approx 1 + \theta \frac{\partial}{\partial_\theta} g(\hat{z}, \theta)|_{\theta=0} = 1 + \theta \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{6}$$

Exercise 1: Please find the explicit matrices for $g(\hat{x},\theta)$ and $g(\hat{y},\theta)$, and find their infinitesimal rotation generators $\frac{\partial}{\partial_\theta} g(\hat{x},\theta)|_{\theta=0}$ and $\frac{\partial}{\partial_\theta} g(\hat{y},\theta)|_{\theta=0}$.

By the physical meaning of rotation, we should have

$$\langle \Psi^g|\Psi^g\rangle = \langle\Psi|\Psi\rangle, \quad \langle \Psi^g|\vec{p}|\Psi^g\rangle = \langle\Psi|g\vec{p}|\Psi\rangle, \quad \langle \Psi^g|\vec{S}|\Psi^g\rangle = \langle\Psi|g\vec{S}|\Psi\rangle. \tag{7}$$

We denote that $|\Psi^g\rangle = D(g)|\Psi\rangle$, and assume that $D(g)$ is a linear unitary operator. We should have

$$\begin{aligned} D(g(\vec{n},0)) &= 1, \\ D^\dagger(g)D(g) &= D(g)D^\dagger(g) = 1, \\ D^\dagger(g)\vec{r}D(g) &= g\vec{r}, \\ D^\dagger(g)\vec{p}D(g) &= g\vec{p} \\ D^\dagger(g)\vec{S}D(g) &= g\vec{S}. \end{aligned} \tag{8}$$

For two successive rotations g_1 and g_2, their net effect is another rotation g whose matrix is defined as $g = g_1 g_2$. Their corresponding rotation operators satisfy the similar relation of product as

$$D(g_1 g_2) = D(g_1)D(g_2). \tag{9}$$

Using the group theory language, $D(g)$'s form a unitary representation for the SO(3) (3D special orthogonal) rotation group.

Next we discuss the relation between the rotation operator and total angular momentum. In the limit of small rotation angle $\theta \to 0$,

$$D(g(\hat{n},\delta\theta))|\Psi(t)\rangle = |\Psi(t)\rangle + \delta\theta \frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}|\Psi(t)\rangle + ..., \tag{10}$$

thus

$$\langle\Psi(t)|D(g)|\Psi(t)\rangle - \langle\Psi(t)|\Psi(t)\rangle = \delta\theta\langle\Psi(t)|\frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}|\Psi(t)\rangle + ... \tag{11}$$

If the space is isotropic around the axis $\hat{n}$, and if $|\Psi(t)\rangle$ is a state vector, then $D(g)|\Psi(t)\rangle$ is also a valid time-dependent state vector, thus the left-hand-side is independent of time. Then $\langle\Psi(t)|\frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}|\Psi(t)\rangle$ is a conserved quantity associated with rotation around the axis $\vec{n}$. It is also easy to show that $\frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}$ is an anti-Hermitian operator. It should be the angular momentum projection to the axis $\vec{n}$ up to a constant α as

$$\frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0} = -\frac{i}{\alpha}\hat{n}\cdot\vec{J}. \tag{12}$$

$\vec{J}$ should be the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. Next we need to determine the constant

α. From $D^\dagger(g)\vec{r}D(g) = g\vec{r}$, we have

$$i\alpha[\hat{n}\cdot\vec{J}, r_i] = \frac{\partial g(\hat{n},\theta)}{\partial\theta}|_{\theta=0,ij} r_j \tag{13}$$

By taking $\vec{n}$ along the z-axis and $r_i = r_x$, we can obtain that $\alpha = \hbar$, and thus

$$D(g(\hat{n},\theta)) = e^{-i\frac{\theta}{\hbar}\hat{n}\cdot\vec{J}} \tag{14}$$

From the Eq. 8 relation $D^\dagger(g)S_iD(g) = g_{ij}S_j$, and take the infinitesimal rotation, we arrive the commutation relation between spin operators

$$[S_i, S_j] = i\varepsilon_{ijk}\hbar S_k. \tag{15}$$

Exercise 2

1. Prove that above statement that $\alpha = \hbar$.
2. Prove Eq. 15.
3. From $D^\dagger(g)L_iD(g) = g_{ij}L_j$, please derive that $[L_i, L_j] = i\varepsilon_{ijk}\hbar L_k$, which is consistent with the direct calculation using the canonical quantization condition.
4. From $D^\dagger(g)p_iD(g) = g_{ij}p_j$, please derive that $[L_i, p_j] = i\varepsilon_{ijk}\hbar p_j$.

3 Pauli matrices for spin-$\frac{1}{2}$ particles

For spin-$\frac{1}{2}$, we can explicitly construct its operators due to its simplicity. The projection of spin along any direction can only take values of $\pm\frac{\hbar}{2}$, thus

$$S_x^2 = S_y^2 = S_z^2 = \frac{1}{4}\hbar^2, \quad S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2. \tag{16}$$

Set $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, such that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$ which are all Hermitian matrices. The satisfy the commutation relation

$$\sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z, \quad \sigma_y\sigma_z - \sigma_z\sigma_y = 2i\sigma_x, \quad \sigma_z\sigma_x - \sigma_x\sigma_z = 2i\sigma_y. \tag{17}$$

A convenient choice of representations of Pauli matrices is

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{18}$$

Pauli matrices have a special properties that other spin matrices do not have, they anti-commute with each other, i.e.,

$$\sigma_i\sigma_j+\sigma_j\sigma_i=2\delta_{ij}, \tag{19}$$

and consequently

$$\sigma_i\sigma_j=\delta_{ij}+i\varepsilon_{ijk}\sigma_k. \tag{20}$$

Pauli matrices are actually the lowest order Clifford algebra. They are also isomorphic to quaternions (the Hamilton number) following the correspondce of

$$i\leftrightarrow -i\sigma_x \quad j\leftrightarrow -i\sigma_y \quad k\leftrightarrow -i\sigma_z. \tag{21}$$

Exercise 3 1) Prove the anti-commutation relation $\sigma_i\sigma_j+\sigma_j\sigma_i=2\delta_{ij}$ which is independent of the concrete representation.

2) Prove that for the rotation operator from the spin part $D_s(n,\theta)=\exp\{-\frac{i}{2}\theta\vec{\sigma}\cdot\vec{n}\}$, it equals to $\cos\frac{\theta}{2}-i(\vec{\sigma}\cdot\vec{n})\sin\frac{\theta}{2}$.

4 Hamiltonian operator for charged particles in the E-M field and gauge invariance

The classic Lagrangian is

$$L(x,\dot{x},t)=\frac{1}{2}m\dot{\vec{r}}^2+\frac{e}{c}\dot{\vec{r}}\cdot\dot{\vec{A}}-e\phi, \tag{22}$$

the canonical momentum is

$$\vec{P}=\frac{\partial L}{\partial\dot{\vec{q}}}=m\dot{\vec{r}}+\frac{e}{c}\vec{A}. \tag{23}$$

Thus

$$H_c(\vec{r},\vec{P})=\vec{P}\cdot\dot{\vec{r}}-L=\frac{(\vec{P}-\frac{e}{c}\vec{A})^2}{2m}+e\phi. \tag{24}$$

Quantum mechanically, we replace the canonical momentum $\vec{P}$, rather than the mechanical momentum, with the operator $-i\hbar\frac{\partial}{\partial x}$. Again it is because of the correspondence principle: In classical mechanics, it is the canonical momentum $\vec{P}$ satisfy the Poisson bracket, not the mechanical momentum. Then for the quantum mechanical Hamiltonian, however, what enters the Hamiltonian is the mechanical momentum which is an physical observable. The canonical momentum is not gauge invariant, and thus is not a physical observable.

$$H = \frac{(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{r}))^2}{2m} + e\phi(\vec{r}). \tag{25}$$

If we expand the above Hamiltonian, we have

$$H = \frac{-\hbar^2\nabla^2}{2m} - \frac{e}{2mc} i\hbar\vec{\nabla}\cdot(\vec{A} - \frac{e}{2mc}\vec{A}\cdot i\hbar\vec{\nabla} + \frac{e^2}{c^2}\frac{\vec{A}^2(\vec{r})}{2m}. \tag{26}$$

The meaning of the second term in the above equation is that for any wavefunction $\psi(\vec{r})$, its effect is $-\frac{i}{2m}\hbar\vec{\nabla}\cdot\{\vec{A}(\vec{r})\psi(\vec{r})\}$. We often use Column like gauge such that $\vec{\nabla}\cdot\vec{A} = 0$, in this case, Eq. 26 is reduced to

$$H = \frac{-\hbar^2\nabla^2}{2m} - \frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla} + \frac{e^2\vec{A}^2(\vec{r})}{2mc^2}. \tag{27}$$

In classic EM, we know that $\vec{A}(\vec{r})$ has gauge redundancy, i.e., for

$$\vec{A}^{'}(\vec{r}) = \vec{A}(\vec{r}) + \nabla f(\vec{r},t), \quad \phi^{'}(\vec{r}) = \phi(\vec{r}) - \frac{1}{c}\frac{\partial}{\partial t} f(\vec{r},t) \tag{28}$$

where $f(\vec{r},t)$ is an arbitrary scale field, $(\vec{A}^{'},\phi^{'})$ and $(\vec{A},\phi)$ represent the same physical electric and magnetic fields. In classic EM, it is not a problem because the equation of motion can be written by using $\vec{E}$ and $\vec{B}$,

$$\vec{F} = m\frac{d^2\vec{r}}{dt^2} = e\vec{E} + e\frac{\vec{v}}{c}\times\vec{B}. \tag{29}$$

The introduction of $\vec{A}$ and ϕ is just a convenience not essential.

However, in quantum mechanics, the concept of force is ill-defined. We have to either use Hamiltonian, or, Lagrangian, both of which can only be expressed by $\vec{A}$ and ϕ not by $\vec{E}$ and $\vec{B}$. The form of Hamiltonian by using $\vec{A}^{'}$ and $\phi^{'}$ is written as

$$H^{'} = \frac{(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}^{'}(\vec{r}))^2}{2m} + e\phi^{'}(\vec{r}). \tag{30}$$

A natural question is: Should $H^{'}$ and H give rise to the same physics?

We can prove that for any solution to the equation

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = H\psi(r,t) \tag{31}$$

with H defined in Eq. 25, we define the a new wavefunction $\psi^{'}(\vec{r},t)$

$$\psi^{'}(\vec{r},t) = e^{\frac{ie}{\hbar c} f(\vec{r},t)} \psi(\vec{r},t) \tag{32}$$

such that it satisfies

$$i\hbar \frac{\partial}{\partial t} \psi^{'}(r,t) = H^{'} \psi^{'}(r,t). \tag{33}$$

Exercise 4 Prove the above statement in Eq. 32 and Eq. 33. Hint: you may need to first verify that

$$(i\hbar \frac{\partial}{\partial t} - e\phi^{'})\psi^{'} = e^{\frac{ie}{\hbar c} f(\vec{r},t)} (i\hbar \frac{\partial}{\partial t} - e\phi)\psi, \tag{34}$$

and you can also find a similar expression with respect to the spatial gradient.

Lecture 6: Pictures

Read Sakurai and Napolitano Chapter 2.1 and 2.2

Both operators and state vectors are unobservable, only the inner products are related to observable quantities. Under the requirement of keeping the inner products invariant, we can use different pictures to formulate the time-evolution in quantum mechanics. They are related to similar transformations.

1 Schrödinger picture

The time evolution is expressed as the evolution of state vectors. The canonical coordinates, momenta, spin do not change with time.

$$|\Psi^S(t)\rangle = T(t,t_0)|\Psi^s(t_0)\rangle. \tag{1}$$

Assume that F^s is an operator for the observable F in the Schrödinger picture, we have its expectation value

$$\overline{F^s} = \langle\Psi^s(t)|F^s|\Psi^s(t)\rangle. \tag{2}$$

If H^s does not depend on t, then $T(t,0) = \exp\{-\frac{i}{\hbar}Ht\}$. If H^s explicitly depend on t, the expression of T is not so simple. According to $\frac{\partial}{\partial t}T(t,0) = -\frac{i}{\hbar}H^s(t)T(t,0)$, we have

$$T(t,0) = 1 + \frac{-i}{\hbar}\int_0^t dt_1 H^s(t_1)T(t_1,0), \tag{3}$$

and by iteration,

$$\begin{aligned}
T(t,0) &= 1 + \frac{-i}{\hbar}\int_0^t dt_1 H^s(t_1) + (\frac{-i}{\hbar})^2\int_0^t dt_1\int_0^{t_1} dt_2 H^s(t_1)H^s(t_2) \\
&+ ... + (\frac{-i}{\hbar})^n\int_0^t dt_1 ...\int_0^{t_{n-1}} dt_n H^s(t_1)H^s(t_2)...H^s(t_n) + ... \\
&= \sum_{n=0}^{+\infty}\frac{1}{n!}(\frac{-i}{\hbar})^n\int_0^t dt_1 ...\int_0^t dt_n \mathcal{T} H^s(t_1)H^s(t_2)...H^s(t_n) \\
&= \mathcal{T}\exp\{\frac{-i}{\hbar}\int_0^t H(t^{'})dt^{'}\}.
\end{aligned} \tag{4}$$

$\mathcal{T}$ is the time-ordered operator. $\mathcal{T}$ is defined as

$$\mathcal{T}H(t_1)H(t_2)...H(t_n) = \sum_p \theta(t_{p_1} > t_{p_2} > ... > t_{p_n})H(t_{p_1})H(t_{p_2})...H(t_{p_n}), \tag{5}$$

where p is a permutation of $1,2,...,n$, and θ-function equals to 1 if the condition $t_{p_1} > t_{p_2} > ... > t_{p_n}$ is satisfied and otherwise 0.

2 Heisenberg picture

We can also fix state vector stationary with time, say, set the state vector in Heisenberg picture as the that of the Schrödinger one at $t = 0$, and let operator to evolve with time:

$$\begin{aligned} |\Psi^H\rangle &= |\Psi^s(0)\rangle, \\ \hat{F}^H(t) &= T^t(t,0)\hat{F}^s T(t,0), \end{aligned} \tag{6}$$

such that

$$\langle\Psi^H|F^H|\Psi^H\rangle = \langle\Psi^s|F^s|\Psi^s\rangle. \tag{7}$$

Actually, F^s can also explicitly depend on time as $F^s(t)$.

Now let us derive the equation of motion of operators. From the Schrödinger equation in which that H^s may explicitly depend on time, $i\hbar\frac{\partial}{\partial t}|\Psi^s(t)\rangle = H^s(t)|\Psi^s(t)\rangle$, we have $i\hbar\frac{\partial}{\partial t}T(t,0)|\Psi^s(0)\rangle = H^s(t)T(t,0)|\Psi^s(0)\rangle$, thus we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}T(t,0) &= H^s(t)T(t,0) \\ -i\hbar\frac{\partial}{\partial t}T^\dagger(t,0) &= T^\dagger(t,0)H^s(t). \end{aligned} \tag{8}$$

Then we have $\frac{d}{dt}F^H(t) = \frac{\partial}{\partial t}T^t(t,0)F^s(t)T(t,0) + T^t(t,0)\frac{\partial}{\partial t}F^s(t)T(t,0) + T^t(t,0)F^s(t)\frac{\partial}{\partial t}T(t,0)$, and then

$$\frac{d}{dt}F^H(t) = \frac{1}{i\hbar}[F^H(t), H^H(t)] + T^\dagger(t,0)\frac{\partial F^s(t)}{\partial t}T(t,0), \tag{9}$$

where $H^H(t) = T^\dagger(t,0)H^s(t)T(t,0)$. In particular, for the canonical coordinate and momentum, we have

$$\begin{aligned} \frac{d}{dt}q_j^H(t) &= \frac{1}{i\hbar}[q_j^H(t), H^H(t)], \\ \frac{d}{dt}p_j^H(t) &= \frac{1}{i\hbar}[p_j^H(t), H^H(t)]. \end{aligned} \tag{10}$$

Example 1) Consider the Hamiltonian of an harmonic oscillator in the Schrödinger picture

$$H^S = \frac{p^{S,2}}{2m} + \frac{1}{2}m\omega^2 x^{S,2}. \tag{11}$$

Then the operators in the Heisenberg picture x^H and p^H can be solved in the following way.

$$\begin{aligned}\frac{d}{dt}x^H(t) &= \frac{1}{i\hbar}[x^H(t),H^H] = \frac{1}{i\hbar}e^{iHt}[x,H^S]e^{-iHt}, \\ \frac{d}{dt}p^H(t) &= \frac{1}{i\hbar}[p^H(t),H^H] = \frac{1}{i\hbar}e^{iHt}[p,H^S]e^{-iHt}. \end{aligned} \tag{12}$$

Using the fact that

$$[x^S,H^S] = \frac{1}{2m}[x,p^{S,2}] = \frac{i\hbar}{m}p^S \tag{13}$$

and

$$[p^S,H^s] = \frac{1}{2}m\omega^2[p^S,x^2] = -i\hbar m\omega^2 x^S, \tag{14}$$

we arrive at

$$\frac{d}{dt}x^H(t) = \frac{p^H(t)}{m}, \quad \frac{d}{dt}p^H(t) = -m\omega^2 x^H(t), \tag{15}$$

the solution will be

$$\begin{aligned} x^H(t) &= x^S\cos\omega t + \frac{p^S}{m\omega}\sin\omega t, \\ p^H(t) &= -m\omega x^S\sin\omega t + p^S\cos\omega t. \end{aligned} \tag{16}$$

Exercise 1 Please prove Eq. 16 for harmonic oscillators by directly using

$$x^H(t) = e^{\frac{i}{\hbar}H^S t}x^S e^{-\frac{i}{\hbar}H^S t}, \quad p^H(t) = e^{\frac{i}{\hbar}H^S t}p^S e^{-\frac{i}{\hbar}H^S t}. \tag{17}$$

Hint: You may use the Baker-Hausdorff lemma in page 95 in Sakurai and Napolitano's book. This formula is proved in my notes in lecture 7.

3 Interaction picture

We decompose the Hamiltonian H^s of the Schrödinger picture into the free part H_0 and the perturbative part V as

$$H^s = H_0 + V, \tag{18}$$

which H_0 is independent of time; V may depend on time. We define that the state vector evolves with time as

$$|\Psi^I(t)\rangle = e^{iH_0t/\hbar}|\Psi^S(t)\rangle = e^{iH_0t/\hbar}T(t,0)|\Psi^S(0)\rangle, \tag{19}$$

and correspondingly the operator

$$F^I(t) = e^{iH_0 t/\hbar} F^s e^{-iH_0 t/\hbar}. \tag{20}$$

In such a convention, we keep the inner product invariant

$$\langle \Psi_A^I(t)|F^I(t)|\Psi_B^I(t)\rangle = \langle \Psi_A^S(t)|F^S(t)|\Psi_B^S(t)\rangle \tag{21}$$

Now let us derive equation of motion, we have

$$\frac{d}{dt}F^I(t) = \frac{1}{i\hbar}[F^I(t), H_0] + e^{iH_0 t/\hbar}\frac{\partial F^s(t)}{\partial t}e^{-iH_0 t/\hbar}. \tag{22}$$

For state vector, we have

$$\begin{aligned}
\frac{\partial}{\partial t}|\Psi^I(t)\rangle &= \frac{i}{\hbar}H_0 e^{iH_0 t/\hbar}|\Psi^s(t)\rangle + e^{iH_0 t/\hbar}\frac{1}{i\hbar}H^S|\Psi^S(t)\rangle \\
&= e^{iH_0 t/\hbar}\frac{i}{\hbar}(H_0 - H^s)e^{-iH_0 t/\hbar}|\Psi^I(t)\rangle = \frac{1}{i\hbar}V^I(t)|\Psi^I(t)\rangle.
\end{aligned} \tag{23}$$

From Eq. 23, we can derive the time-evolution operator $U(t,t_0)$ in the interaction picture as

$$\begin{aligned}
|\Psi^I(t)\rangle &= U(t,t_0)|\Psi^I(t_0)\rangle, \\
U(t,t_0) &= \mathcal{T}\exp\{-\frac{i}{\hbar}\int_{t_0}^{t} dt' V^I(t')\}.
\end{aligned} \tag{24}$$

Exercise 2

1. Prove Eq. 22 of $\frac{d}{dt}F^I(t)$.
2. Prove the above expression of $U(t,t_0)$.

Example Let us consider a perturbed Harmonic potential

$$H = H_0 + V(x), \tag{25}$$

where $H_0 = p^2/2m + \frac{1}{2}m\omega^2 x^2$ and $V(x)$ is a small perturbation. In the interaction picture, we have

$$\begin{aligned}
x^I(t) = e^{\frac{i}{\hbar}H_0 t} x e^{-\frac{i}{\hbar}H_0 t} &= x\cos\omega t + \frac{p}{m\omega}\sin\omega t, \\
p^I(t) = e^{\frac{i}{\hbar}H_0 t} p e^{-\frac{i}{\hbar}H_0 t} &= -m\omega x\sin\omega t + p\cos\omega t,
\end{aligned} \tag{26}$$

and thus

$$V^I(t) = V(x^I(t)). \tag{27}$$

The time-evolution operator for the state vectors are

$$U(t,t_0) = \mathcal{T} \exp\{-\frac{i}{\hbar}\int_{t_0}^{t} dt V(x^I(t))\}. \tag{28}$$