AQM1-2

chp2: Quantum Dynamics

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فصل دوم

TIME EVOLUTION AND THE SCHRÖDINGER EQUATION

$$|\alpha, t_0\rangle = |\alpha\rangle \xrightarrow{\text{time evolution}} |\alpha, t_0; t\rangle.$$

time-evolution operator $\mathscr{U}(t, t_0)$:

$$\boxed{|\alpha, t_0; t\rangle = \mathscr{U}(t, t_0)|\alpha, t_0\rangle.}$$

$$|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0)|a'\rangle.$$

at some later time, $|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t)|a'\rangle.$

$$|c_{a'}(t)| \neq |c_{a'}(t_0)|.$$

$$\sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2$$

fundamental properties of the $\mathscr{U}$ operator

$$\langle \alpha, t_0 | \alpha, t_0 \rangle = 1 \Rightarrow \langle \alpha, t_0; t | \alpha, t_0; t \rangle = 1$$

$$\mathscr{U}^\dagger(t, t_0)\mathscr{U}(t, t_0) = 1$$

$$\mathscr{U}(t_2, t_0) = \mathscr{U}(t_2, t_1)\mathscr{U}(t_1, t_0), \quad (t_2 > t_1 > t_0)$$

$$\lim_{dt \to 0} \mathscr{U}(t_0 + dt, t_0) = 1$$

be unitary: $\mathscr{T}^\dagger(d\mathbf{x}')\mathscr{T}(d\mathbf{x}') = 1.$

$$\mathscr{T}(d\mathbf{x}'')\mathscr{T}(d\mathbf{x}') = \mathscr{T}(d\mathbf{x}' + d\mathbf{x}'').$$

$$\boxed{\mathscr{T}(-d\mathbf{x}') = \mathscr{T}^{-1}(d\mathbf{x}').}$$

$$\lim_{d\mathbf{x}' \to 0} \mathscr{T}(d\mathbf{x}') = 1$$

all these requirements are satisfied by

$$\mathscr{U}(t_0 + dt, t_0) = 1 - i\Omega\, dt \qquad (2.1.15)$$

where Ω is a Hermitian operator,* $\Omega^\dagger = \Omega$

$$\mathscr{U}(t_0 + dt_1 + dt_2, t_0) = \mathscr{U}(t_0 + dt_1 + dt_2, t_0 + dt_1)\mathscr{U}(t_0 + dt_1, t_0)$$

$$\mathscr{U}^\dagger(t_0 + dt, t_0)\mathscr{U}(t_0 + dt, t_0) = (1 + i\Omega^\dagger\, dt)(1 - i\Omega\, dt) \simeq 1$$

$$\mathscr{T}(d\mathbf{x}') = 1 - i\mathbf{K}\cdot d\mathbf{x}',$$

The operator Ω has the dimension of frequency or inverse time. Is there any familiar observable with the dimension of frequency? We recall that in the old quantum theory, angular frequency ω is postulated to be related to energy by the Planck-Einstein relation

$$E = \hbar\omega. \tag{2.1.19}$$

Let us now borrow from classical mechanics the idea that the Hamiltonian is the generator of time evolution (Goldstein 1980, 407–8). It is then natural to relate Ω to the Hamiltonian operator H:

$$\Omega = \frac{H}{\hbar}. \tag{2.1.20}$$

$$\mathcal{U}(t_0 + dt, t_0) = 1 - \frac{iH\,dt}{\hbar}, \tag{2.1.21}$$

کمیت توصیف کننده حالت سیستم		مولد تغییر	
مختصات، مکان یک ذره	x	تکانه	P
زمان	t	انرژی، هامیلتونی	H
جهت گیری ذره (یا سیستم)	?	چرخش	S، L

The Schrödinger Equation

$$\mathscr{U}(t+dt, t_0) - \mathscr{U}(t, t_0) = -i\left(\frac{H}{\hbar}\right) dt\, \mathscr{U}(t, t_0), \qquad (2.1.24)$$

Schrödinger equation for the time-evolution operator

$$\boxed{i\hbar \frac{\partial}{\partial t} \mathscr{U}(t, t_0) = H \mathscr{U}(t, t_0).} \qquad (2.1.25)$$

$$\longrightarrow \quad i\hbar \frac{\partial}{\partial t} \mathscr{U}(t, t_0)|\alpha, t_0\rangle = H \mathscr{U}(t, t_0)|\alpha, t_0\rangle.$$

Schrödinger equation for the state ket

$$\boxed{i\hbar \frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle,} \qquad (2.1.27)$$

If we are given $\mathscr{U}(t, t_0)$ and, in addition, know how $\mathscr{U}(t, t_0)$ acts on the initial state ket $|\alpha, t_0\rangle$, it is not necessary to bother with the Schrödinger equation for the state ket (2.1.27). All we have to do is apply $\mathscr{U}(t, t_0)$ to $|\alpha, t_0\rangle$; in this manner we can obtain a state ket at any t.

$$\boxed{i\hbar \frac{\partial}{\partial t} \mathscr{U}(t, t_0) = H \mathscr{U}(t, t_0)}$$

Case 1. The Hamiltonian operator is independent of time.

$$\mathscr{U}(t, t_0) = \exp\left[\frac{-iH(t-t_0)}{\hbar}\right]. \tag{2.1.28}$$

To prove this let us expand the exponential as follows:

$$\exp\left[\frac{-iH(t-t_0)}{\hbar}\right] = 1 - \frac{iH(t-t_0)}{\hbar} + \left[\frac{(-i)^2}{2}\right]\left[\frac{H(t-t_0)}{\hbar}\right]^2 + \cdots. \tag{2.1.29}$$

Because the time derivative of this expansion is given by

$$\frac{\partial}{\partial t}\exp\left[\frac{-iH(t-t_0)}{\hbar}\right] = \frac{-iH}{\hbar} + \left[\frac{(-i)^2}{2}\right] 2\left(\frac{H}{\hbar}\right)^2 (t-t_0) + \cdots, \tag{2.1.30}$$

$$\lim_{N\to\infty}\left[1 - \frac{(iH/\hbar)(t-t_0)}{N}\right]^N = \exp\left[\frac{-iH(t-t_0)}{\hbar}\right]. \tag{2.1.31}$$

Case 2. The Hamiltonian operator H is time-dependent but the H's at different times commute.

$$\mathscr{U}(t, t_0) = \exp\left[-\left(\frac{i}{\hbar}\right)\int_{t_0}^{t} dt' H(t')\right]. \tag{2.1.32}$$

Case 3. The H's at different times do *not* commute.

$$\mathscr{U}(t, t_0) = 1 + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1) H(t_2) \cdots H(t_n), \tag{2.1.33}$$

which is sometimes known as the **Dyson series**, after F. J. Dyson, who developed a perturbation expansion of this form in quantum field theory.

Energy Eigenkets

To be able to evaluate the effect of the time-evolution operator (2.1.28) on a general initial ket $|\alpha\rangle$, we must first know how it acts on the base kets used in expanding $|\alpha\rangle$. This is particularly straightforward if the base kets used are eigenkets of A such that

$$[A, H] = 0; \tag{2.1.34}$$

then the eigenkets of A are also eigenkets of H, called **energy eigenkets**, whose eigenvalues are denoted by $E_{a'}$:

$$H|a'\rangle = E_{a'}|a'\rangle. \tag{2.1.35}$$

We can now expand the time-evolution operator in terms of $|a'\rangle\langle a'|$. Taking $t_0 = 0$ for simplicity, we obtain

$$\exp\left(\frac{-iHt}{\hbar}\right) = \sum_{a'}\sum_{a''}|a''\rangle\langle a''|\exp\left(\frac{-iHt}{\hbar}\right)|a'\rangle\langle a'| = \sum_{a'}|a'\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)\langle a'|. \tag{2.1.36}$$

$$\boxed{\exp\left(\frac{-iHt}{\hbar}\right) = \sum_{a'}|a'\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)\langle a'|.}$$

As an example,

$$|\alpha\rangle = |\alpha, t_0 = 0\rangle = \sum_{a'} |a'\rangle \boxed{\langle a'|\alpha\rangle} = \sum_{a'} c_{a'} |a'\rangle .$$

$$|\alpha, t\rangle = |\alpha, t_0 = 0; t\rangle = \exp\left(\frac{-iHt}{\hbar}\right)|\alpha\rangle = \sum_{a'} |a'\rangle \boxed{\langle a'|\alpha\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right)}.$$

$$\longrightarrow \quad c_{a'}(t=0) \to c_{a'}(t) = c_{a'}(t=0)\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

$$|\alpha\rangle = |a'\rangle \quad \longrightarrow \quad |\alpha, t\rangle = |a'\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right),$$

so if the system is initially a simultaneous eigenstate of A and H, it remains so at all times. The most that can happen is the phase modulation, $\exp(-iE_{a'}t/\hbar)$. It is in this sense that an observable compatible with H [see (2.1.34)] is a *constant of the motion*.

In the foregoing discussion the basic task in quantum dynamics is reduced to finding an observable that commutes with H and evaluating its eigenvalues. Once that is done, we expand the initial ket in terms of the eigenkets of that observable and just apply the time-evolution operator. This last step merely amounts to changing the phase of each expansion coefficient, as indicated by (2.1.39).

Even though we worked out the case where there is just one observable A that commutes with H, our considerations can easily be generalized when there are several mutually compatible observables all also commuting with H:

$$[A,B]=[B,C]=[A,C]=\cdots=0,$$
$$[A,H]=[B,H]=[C,H]=\cdots=0. \tag{2.1.42}$$

Using the collective index notation of Section 1.4 [see (1.4.37)], we have

$$\exp\left(\frac{-iHt}{\hbar}\right)=\sum_{K'}|K'\rangle\exp\left(\frac{-iE_{K'}t}{\hbar}\right)\langle K'|, \tag{2.1.43}$$

where $E_{K'}$ is uniquely specified once $a', b', c', \ldots$ are specified. It is therefore of fundamental importance to find *a complete set of mutually compatible observables that also commute with* H. Once such a set is found, we express the initial ket as a superposition of the simultaneous eigenkets of $A, B, C, \ldots$ and H. The final step is just to apply the time-evolution operator, written as (2.1.43). In this manner we can solve the most general initial-value problem with a time-independent H.

وابستگی زمانیِ مقادیر چشمداشتی

فرض کنید A و H جابجا می شوند و ما قصد داریم مقدار چشمداشتی عملگر دیگری مثل B را که لزوما با A و H جابجا نمی شود محاسبه کنیم

$$|a', t_0 = 0; t\rangle = \mathscr{U}(t, 0)|a'\rangle \qquad (2.1.44)$$

$$\begin{aligned}
\langle B \rangle &= (\langle a'|\mathscr{U}^\dagger(t,0)) \cdot B \cdot (\mathscr{U}(t,0)|a'\rangle) \\
&= \langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right) B \exp\left(\frac{-iE_{a'}t}{\hbar}\right)|a'\rangle \\
&= \langle a'|B|a'\rangle, \qquad (2.1.45)
\end{aligned}$$

which is *independent of t*.

نتیجه: مقدار چشمداشتی یک مشاهده پذیر وقتی در **ویژه حالت های انرژی** محاسبه می شود، با زمان تغییر نمی کند (مستقل از زمان است). به همین خاطر ویژه حالت انرژی را حالت مانا (Stationary state) می گویند.

وابستگی زمانیِ مقادیر چشمداشتی

اگر مقدار چشمداشتی را در حالت غیرِ مانا (که از برهم نهی ویژه حالت های انرژی حاصل می شود) محاسبه کنیم:

$$|\alpha, t_0 = 0\rangle = \sum_{a'} c_{a'} |a'\rangle. \quad (2.1.46)$$

$$\langle B \rangle = \left[\sum_{a'} c_{a'}^* \langle a' | \exp\left(\frac{iE_{a'}t}{\hbar} \right) \right] \cdot B \cdot \left[\sum_{a''} c_{a''} \exp\left(\frac{-iE_{a''}t}{\hbar} \right) |a''\rangle \right]$$

$$= \sum_{a'} \sum_{a''} c_{a'}^* c_{a''} \langle a' | B | a'' \rangle \exp\left[\frac{-i(E_{a''} - E_{a'})t}{\hbar} \right]. \quad (2.1.47)$$

مقدار چشمداشتی یک جمله نوسانی خواهد داشت، که فرکانس زاویه ای آن از رابطه فرکانسی بوهر طبعیت می کند:

$$\omega_{a''a'} = \frac{(E_{a''} - E_{a'})}{\hbar} \quad (2.1.48)$$

حرکت تقدیمی اسپین

تصویر شرودینگر / هایزنبرگ / دیراک

در رهیافتی که پیشتر معرفی کردیم؛ پیشرویِ زمان با اثر دادن عملگر تحول زمانی روی کت های حالت توصیف شد. این رهیافت را **تصویر شرودینگر** می گوییم.
رهیافت دیگری هم وجود دارد که در آن به جای اینکه کت های حالت با زمان متحول شوند، عملگرها با زمان متحول می شوند. این رهیافت به **تصویر هایزنبرگ** معروف است.

نکته – تغییر کتِ پایه، کتِ حالت را تغییر نمی دهد. (*درباره ی معنی اش فکر کنید!*)

اگر عملگرهای یکانی روی حالت اثر کنند، رابطه ی زیر برقرار است.

$$|\alpha\rangle \rightarrow U|\alpha\rangle$$

where U may stand for $\mathscr{T}(d\mathbf{x})$ or $\mathscr{U}(t, t_0)$

چون $UU^\dagger = 1$

$$\langle\beta|\alpha\rangle \rightarrow \langle\beta|U^\dagger U|\alpha\rangle = \langle\beta|\alpha\rangle$$

$$\langle \beta | \alpha \rangle \rightarrow \langle \beta | U^\dagger U | \alpha \rangle = \langle \beta | \alpha \rangle$$

$$\langle \beta | X | \alpha \rangle \rightarrow (\langle \beta | U^\dagger) \cdot X \cdot (U | \alpha \rangle) = \langle \beta | U^\dagger X U | \alpha \rangle$$

$$(\langle \beta | U^\dagger) \cdot X \cdot (U | \alpha \rangle) = \langle \beta | \cdot (U^\dagger X U) \cdot | \alpha \rangle. \tag{2.2.4}$$

Approach 1:

$$|\alpha\rangle \rightarrow U|\alpha\rangle, \quad \text{with operators unchanged,} \tag{2.2.5a}$$

Approach 2:

$$X \rightarrow U^\dagger X U, \quad \text{with state kets unchanged.} \tag{2.2.5b}$$

مثال

نشان دهید که مقدار چشمداشتیِ عملگر x در کت حالتِ آلفا در تصویر شرودینگر و تصویر هایزنبرگ یکی خواهد شد.

(یعنی اگر عملگر انتقال در فضا را به کت حالت اثر دهیم یا به عملگر مکان اثر دهیم، مقدار چشمداشتی های حاصل از اثر این عملگر یکی خواهند شد).

$$|\alpha\rangle \to \left(1 - \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)|\alpha\rangle$$

$$\mathbf{x} \to \left(1 + \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\mathbf{x}\left(1 - \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)$$

کت حالت و مشاهده پذیرها در تصویر هایزنبرگ

$$\mathscr{U}(t, t_0 = 0) \equiv \mathscr{U}(t) = \exp\left(\frac{-iHt}{\hbar}\right)$$

$$A^{(H)}(t) \equiv \mathscr{U}^\dagger(t) A^{(S)} \mathscr{U}(t)$$ $$A^{(H)}(0) = A^{(S)}$$

$$|\alpha, t_0 = 0; t\rangle_H = |\alpha, t_0 = 0\rangle$$ $$|\alpha, t_0 = 0; t\rangle_S = \mathscr{U}(t)|\alpha, t_0 = 0\rangle$$

The expectation value $\langle A\rangle$ is obviously the same in both pictures:

$$\begin{aligned} {}_S\langle\alpha, t_0 = 0; t|A^{(S)}|\alpha, t_0 = 0; t\rangle_S &= \langle\alpha, t_0 = 0|\mathscr{U}^\dagger A^{(S)} \mathscr{U}|\alpha, t_0 = 0\rangle \\ &= {}_H\langle\alpha, t_0 = 0; t|A^{(H)}(t)|\alpha, t_0 = 0; t\rangle_H. \end{aligned} \tag{2.2.14}$$

معادله حرکت در تصویر هایزنبرگ

$$\frac{dA^{(H)}}{dt} = \frac{\partial \mathscr{U}^\dagger}{\partial t} A^{(S)} \mathscr{U} + \mathscr{U}^\dagger A^{(S)} \frac{\partial \mathscr{U}}{\partial t}$$

$$= -\frac{1}{i\hbar} \mathscr{U}^\dagger H \mathscr{U} \mathscr{U}^\dagger A^{(S)} \mathscr{U} + \frac{1}{i\hbar} \mathscr{U}^\dagger A^{(S)} \mathscr{U} \mathscr{U}^\dagger H \mathscr{U}$$

$$= \frac{1}{i\hbar} [A^{(H)}, \mathscr{U}^\dagger H \mathscr{U}], \qquad (2.2.15)$$

where we have used [see (2.1.25)]

$$\frac{\partial \mathscr{U}}{\partial t} = \frac{1}{i\hbar} H \mathscr{U}, \qquad (2.2.16a)$$

$$\frac{\partial \mathscr{U}^\dagger}{\partial t} = -\frac{1}{i\hbar} \mathscr{U}^\dagger H. \qquad (2.2.16b)$$

$$H^{(H)} = \mathscr{U}^\dagger H \mathscr{U} \qquad (2.2.17)$$

$\mathscr{U}$ and H obviously commute; as a result,

$$\mathscr{U}^\dagger H \mathscr{U} = H, \qquad (2.2.18)$$

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H] \qquad (2.2.19)$$

Heisenberg equation of motion

(Goldstein 1980, 405–6) $$\frac{dA}{dt} = [A, H]_{\text{classical}} \qquad (2.2.20)$$

$$\frac{[\ ,\ ]}{i\hbar} \rightarrow [\ ,\ ]_{\text{classical}}$$

هامیلتونی در کوانتم

مهم ترین کاری که برای حل مساله یک سیستم کوانتمی باید انجام شود، نوشتن هامیلتونی برای این سیستم است.

برای سیستم های فیزیکی که مشابه کلاسیکی دارند، هامیلتونی را مثل هامیلتونی کلاسیک می نویسیم. فقط متوجه هستیم که مکان و تکانه عملگر هستند.

نکته مهم دیگر این است که معادل کوانتمی را طوری می سازیم که عملگر هامیلتونی، هرمیتی باشد!

we write the quantum-mechanical analogue of the classical product xp as $\frac{1}{2}(xp + px)$.

اگر سیستمی معادل کلاسیکی نداشته باشد، شکل هامیلتونی را باید حدس بزنیم و شکل های مختلفی را امتحان کنیم تا نتایج با نتایج آزمایشگاهی یکسان شود.

دو تا فرمول مفید:

$$[x_i, F(\mathbf{p})] = i\hbar \frac{\partial F}{\partial p_i} \qquad (2.2.23a)$$

$$[p_i, G(\mathbf{x})] = -i\hbar \frac{\partial G}{\partial x_i}, \qquad (2.2.23b)$$

تمرین (برای خودتان)

معادله ی حرکت یک ذره با هامیلتونی مقابل را با استفاده از تصویر هایزنبرگ بنویسید.

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$$

جواب:

$$m\frac{d^2\mathbf{x}}{dt^2} = -\nabla V(\mathbf{x})$$

قضیه ارنفست

This is the quantum-mechanical analogue of Newton's second law. By taking the expectation values of both sides with respect to a Heisenberg state ket that does *not* move with time, we obtain

$$\boxed{m\frac{d^2}{dt^2}\langle \mathbf{x}\rangle = \frac{d\langle \mathbf{p}\rangle}{dt} = -\langle \nabla V(\mathbf{x})\rangle .} \tag{2.2.36}$$

This is known as the **Ehrenfest theorem** after P. Ehrenfest, who derived it in 1927 using the formalism of wave mechanics. When written in this expectation form, its validity is independent of whether we are using the Heisenberg or the Schrödinger picture; after all, the expectation values are the same in the two pictures. In contrast, the operator form (2.2.35) is meaningful only if we understand **x** and **p** to be Heisenberg-picture operators.

یک نکته ظریف: مقدار متوسط های کوانتمی مثل کلاسیک رفتار می کنند (البته با یک ملاحظاتی!). *جایی که مشتق گیری ها نسبت به عملگر ها باشد، مشتق گیری هم نسبت به مقدار متوسط انجام گیرد!*

$$\left\langle \frac{\partial H}{\partial p}\right\rangle = \frac{\partial}{\partial\langle p\rangle} H(\langle p\rangle,\langle q\rangle,t)$$

تحول زمانی کت پایه !!

در تصویر شرودینگر عملگرها تغییر نمی کنند، پس کت های پایه هم نباید تغییر کنند. اما در تصویر هایزنبرگ باید ببینیم چه اتفاقی برای پایه ها می افتد.

$$A|a'\rangle = a'|a'\rangle \qquad A^{(H)}(t) = \mathscr{U}^\dagger A(0)\mathscr{U}$$

$$\mathscr{U}^\dagger A(0)\mathscr{U}\mathscr{U}^\dagger|a'\rangle = a'\mathscr{U}^\dagger|a'\rangle$$

$$i\hbar\frac{\partial}{\partial t}\mathscr{U}(t,t_0) = H\mathscr{U}(t,t_0)$$

$$A^{(H)}\left(\mathscr{U}^\dagger|a'\rangle\right) = a'\left(\mathscr{U}^\dagger|a'\rangle\right)$$

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H]$$

$$\boxed{|a',t\rangle_H = \mathscr{U}^\dagger|a'\rangle} \qquad \boxed{i\hbar\frac{\partial}{\partial t}|a',t\rangle_H = -H|a',t\rangle_H}$$

$$c_{a'}(t) = \underbrace{\langle a'|}_{\text{base bra}} \cdot \underbrace{\left(\mathscr{U}|\alpha, t_0=0\rangle\right)}_{\text{state ket}} \quad \text{(the Schrödinger picture)} \quad (2.2.44a)$$

$$c_{a'}(t) = \underbrace{\left(\langle a'|\mathscr{U}\right)}_{\text{base bra}} \cdot \underbrace{|\alpha, t_0=0\rangle}_{\text{state ket}} \quad \text{(the Heisenberg picture)}. \quad (2.2.44b)$$