第五章 时间演化：三种绘景

讨论：

a. 时间不是算符，仅为一参量

b. 描述不同时刻态/算符间的关系

c. 存在多种等价的描述方式（绘景）

1. Schrodiger 方程

$i\hbar\partial_t|\psi\rangle=\hat{H}|\psi\rangle$

若 $|\psi\rangle$ 为 $\hat{H}$ 的本征态，满足 $\hat{H}|\psi\rangle=E|\psi\rangle$ $\Rightarrow$ $i\hbar\partial_t|\psi\rangle=E|\psi\rangle$ $\Rightarrow$ $|\psi(t)\rangle=e^{-\frac{iEt}{\hbar}}|\psi(0)\rangle$ 定态

坐标表象下：$i\hbar\partial_t\psi(r,t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]\psi(r,t)$ $\Leftrightarrow$ $\langle r|i\hbar\partial_t|\psi\rangle=\int d^3r'\langle r|\hat{H}|r'\rangle\langle r'|\psi\rangle$

缩写

令 $\psi(r,t)=\psi(r)T(t)$

$\Rightarrow$ $i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt}=\frac{1}{\psi(r)}\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]\psi(r)\triangleq E$

$\Rightarrow$ $T(t)=e^{-\frac{iEt}{\hbar}}$ $\Rightarrow$ $\begin{cases}\psi(r,t)=e^{-\frac{iEt}{\hbar}}\psi(r)\\ \left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]\psi(r)=E\psi(r)\end{cases}$

定态的性质：（设 $\hat{H}$ 不显含时）

任意不含时的力学量在定态下的期望值与测量值几率分布不随时变化

$\begin{cases}\langle\psi(t)|\hat{A}|\psi(t)\rangle=\langle\psi(t=0)|\hat{A}|\psi(t=0)\rangle\\ \text{在定态 }|\psi\rangle\text{ 上，测得 }A_n\text{ 的几率为 }|\langle\psi_n|\psi\rangle|^2=|\langle\psi_n|e^{-\frac{iEt}{\hbar}}|\psi(t=0)\rangle|^2=|\langle\psi_n|\psi(t=0)\rangle|^2\end{cases}$

2. 任意态的时间演化

$\{|\psi_n\rangle\}$ 基 在 $\hat{H}$ 不含时条件下：$|\psi(t)\rangle=\sum_n C_n(t)|\psi_n\rangle$

$\Rightarrow$ $i\hbar\sum_n\partial_t C_n(t)|\psi_n\rangle=\sum_n C_n(t)E_n|\psi_n\rangle$

$\xRightarrow{\langle\psi_n|}$ $i\hbar\partial_t C_n(t)=C_n(t)E_n$ （关于系数的方程）

$\Rightarrow$ $C_n(t)=e^{-\frac{iE_nt}{\hbar}}C_n(0)$

$\Rightarrow$ $|\psi(t)\rangle=\sum_n e^{-\frac{iE_nt}{\hbar}}C_n(0)|\psi_n\rangle$

步骤：① 求 $\hat{H}$ 的本征问题 $\{|\psi_n\rangle\}$ $\{E_n\}$

② 用 $\{|\psi_n\rangle\}$ 展开 $|\psi(0)\rangle$

③ 加上演化系数

3. 时间演化算符　　0时刻 $\longrightarrow$ t时刻

令 $|\psi(t)\rangle = \hat{U}|\psi(0)\rangle$　　$\hat{U}(t)$

$\Rightarrow$ $i\hbar\frac{\partial}{\partial t}\hat{U}|\psi(0)\rangle = \hat{H}\hat{U}|\psi(0)\rangle$

$\overset{\forall|\psi(0)\rangle}{\Longrightarrow}$ $i\hbar\frac{\partial}{\partial t}\hat{U} = \hat{H}\hat{U}$　　如$\hat{H}$不显含时，则　$\hat{U} = e^{-i\frac{\hat{H}t}{\hbar}}$

(S方程等价形式)

$\hat{U}|\psi\rangle = \hat{U}\sum_n C_n|\psi_n\rangle = \sum_n C_n e^{-\frac{iE_nt}{\hbar}}|\psi_n\rangle$

$f(\hat{A})|\psi_n\rangle = f(E_n)|\psi_n\rangle$　　$\overset{?}{=} \sum_n C_n e^{-\frac{iE_nt}{\hbar}}|\psi_n\rangle$

可以发现和上面方法结果一致

prop. ① $\hat{U}\hat{U}^{+} = \hat{I}$　　$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\psi(0)\rangle = 1 = \langle\psi(0)|\hat{U}^{+}\hat{U}|\psi(0)\rangle$

幺正算符(不改变模长)

反演算符 $\hat{U}^{+}(t)$　　$\hat{U}^{+}(t)|\psi(t)\rangle = |\psi(0)\rangle$

② $\hat{U}^{+} = e^{i\frac{\hat{H}t}{\hbar}}$　　量子态在$\hat{H}$驱动下随时演化，且时间演化可逆

* $\hat{H}$含时？　$\hat{U} = \int_0^t \left(-\frac{i}{\hbar}\right)\hat{H}(t')\hat{U}(t')dt' + \hat{I}$　　迭代形式解

$\hat{U} = \hat{I} + \int_0^t \left(-\frac{i}{\hbar}\right)\hat{H}(t')dt' + \int_0^t\int_0^t dt'dt\, \hat{H}(t')\hat{H}(t) + \cdots$

$= T e^{-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'}$　　若不同时刻$\hat{H}$对易，则 $\hat{U} = e^{-\frac{i}{\hbar}\int_0^t \hat{H}(t)dt}$

编时算符

例：期望值的时间演化

$\frac{d}{dt}\left(\langle\psi(t)|\hat{A}|\psi(t)\rangle\right) = \left(\frac{\partial}{\partial t}\langle\psi(t)|\right)\hat{A}|\psi(t)\rangle + \langle\psi(t)|\hat{A}\left(\frac{\partial}{\partial t}|\psi(t)\rangle\right) + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle$

代入 $\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{1}{i\hbar}\hat{H}|\psi(t)\rangle$，$\frac{\partial}{\partial t}\langle\psi(t)| = -\frac{1}{i\hbar}\langle\psi(t)|\hat{H}$

原式 $= -\frac{1}{i\hbar}\langle\psi(t)|\hat{H}\hat{A}|\psi(t)\rangle + \frac{1}{i\hbar}\langle\psi(t)|\hat{A}\hat{H}|\psi(t)\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle_\psi$

$= \frac{1}{i\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle_\psi$

$\Rightarrow i\hbar\frac{\partial}{\partial t}\langle\hat{A}\rangle_\psi = \langle[\hat{A},\hat{H}]\rangle_\psi + \langle\frac{\partial\hat{A}}{\partial t}\rangle_\psi$　　Ehrenfest关系

例．在某基组下，$\hat{H}$的矩阵表示为 $\begin{pmatrix} 0 & \frac{A}{2} \\ \frac{A}{2} & 0 \end{pmatrix}$，初态为 $\begin{pmatrix}1\\0\end{pmatrix}$，求t时刻体系状态

法一：① $\hat{H}$的本征问题　$E_1 = \frac{A}{2}$　　$E_2 = -\frac{A}{2}$

$\frac{\sqrt{2}}{2}\begin{pmatrix}1\\1\end{pmatrix}$　　$\frac{\sqrt{2}}{2}\begin{pmatrix}1\\-1\end{pmatrix}$

② 展开

$\begin{pmatrix}1\\0\end{pmatrix} = \frac{\sqrt{2}}{2}\left[\frac{\sqrt{2}}{2}\begin{pmatrix}1\\1\end{pmatrix} + \frac{\sqrt{2}}{2}\begin{pmatrix}1\\-1\end{pmatrix}\right]$

③ 演化系数

$$\frac{1}{2}e^{\frac{iAt}{2\hbar}}\begin{pmatrix}1\\1\end{pmatrix}+\frac{1}{2}e^{\frac{iAt}{2\hbar}}\begin{pmatrix}1\\-1\end{pmatrix}=\begin{pmatrix}\cos\frac{At}{2\hbar}\\-i\sin\frac{At}{2\hbar}\end{pmatrix}$$ → 几率振荡 含时分布

光子耦合原子能级

法二：$\hat{u}|\psi(0)\rangle=e^{-\frac{i\hat{H}t}{\hbar}}|\psi(0)\rangle$

$$\Rightarrow e^{-i\begin{pmatrix}0&\frac{A}{2}\\\frac{A}{2}&0\end{pmatrix}t/\hbar}\begin{pmatrix}1\\0\end{pmatrix}$$

表象变换：

旧基	$\frac{\sqrt{2}}{2}\begin{pmatrix}1\\1\end{pmatrix}$	$\frac{\sqrt{2}}{2}\begin{pmatrix}1\\-1\end{pmatrix}$	G
新基	$\begin{pmatrix}1\\0\end{pmatrix}$	$\begin{pmatrix}0\\1\end{pmatrix}$	F

$$S=\begin{pmatrix}(1\ 0)\frac{\sqrt{2}}{2}\begin{pmatrix}1\\1\end{pmatrix} & (1\ 0)\frac{\sqrt{2}}{2}\begin{pmatrix}1\\-1\end{pmatrix}\\(0\ 1)\frac{\sqrt{2}}{2}\begin{pmatrix}1\\1\end{pmatrix} & (0\ 1)\frac{\sqrt{2}}{2}\begin{pmatrix}1\\-1\end{pmatrix}\end{pmatrix}=\frac{\sqrt{2}}{2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$ 其实就这 $(\vec{x_1}\ \vec{x_2})$

$$\Rightarrow S e^{-i\begin{pmatrix}\frac{A}{2}&0\\0&-\frac{A}{2}\end{pmatrix}t/\hbar}S^{+}\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}\cos\frac{At}{2\hbar}\\-i\sin\frac{At}{2\hbar}\end{pmatrix}$$

$LHL^{-1}=H$ $[H,L]=0$

$[\hat{P},\hat{H}]=0\Rightarrow L$ 一 平移算符

* 守恒量：不显含时且与 $\hat{H}$ 对易的力学量

(对称性与守恒量)

prop：无论体系处于什么态，守恒量的期望值与测量几率分布不随时改变

prop：守恒量与 $\hat{H}$ 有共同本征态 $\{|\psi_n\rangle\}$

$$|\psi\rangle=\sum_n C_n e^{-\frac{iE_nt}{\hbar}}|\psi_n\rangle$$ $|A_n,E_n\rangle$

4. 三种绘景 (picture) —— 态与算符都不可观测，所以可以用别的框架描述可观测量演化

(含时演化就化)
除了方程形式都一样

a. Schrodiger 绘景

态 $|\psi(t)\rangle$ 含时演化 → S方程

力学量 $\hat{A}$ 不含时演化

} 可观测量

b. Heisenberg 绘景

要求态不演化，力学量演化，但必须 $\langle\hat{A}\rangle=\langle\psi|\hat{A}|\psi\rangle$ 不变

$$\left.\begin{array}{l}|\psi(0)\rangle_S=|\psi\rangle_H\\|\psi(t)\rangle_S=\hat{u}|\psi(0)\rangle_S\end{array}\right\}\ |\psi\rangle_H=\hat{u}^{+}|\psi(t)\rangle_S$$

$$\Rightarrow {}_H\langle\psi|\hat{A}_H|\psi\rangle_H={}_S\langle\psi(t)|\hat{A}_S|\psi(t)\rangle_S$$
$$\shortparallel$$
$${}_S\langle\psi(t)|\hat{u}\hat{A}_H\hat{u}^{+}|\psi(t)\rangle_S$$

$\Rightarrow$ 要求 $\hat{A}_S=\hat{u}\hat{A}_H\hat{u}^{+}$ 即 $\hat{A}_H=\hat{u}^{+}\hat{A}_S\hat{u}$

算符的动力学方程：

$$\frac{d\hat{A}_H}{dt}=\left(\frac{d}{dt}\hat{u}^{+}\right)\hat{A}_S\hat{u}+\hat{u}^{+}\frac{d\hat{A}_S}{dt}\hat{u}+\hat{u}^{+}\hat{A}_S\frac{d\hat{u}}{dt}$$

由S方程等价形式：$i\hbar\frac{d}{dt}\hat{U}=\hat{H}\hat{U} \Rightarrow \frac{d}{dt}\hat{U}=-i\frac{\hat{H}\hat{U}}{\hbar}$

代入得 $\frac{d\hat{A}_H}{dt}=\frac{i}{\hbar}\hat{U}^+\hat{H}\hat{A}_S\hat{U}+\hat{U}^+\left(\frac{\partial\hat{A}_S}{\partial t}\right)\hat{U}-\frac{i}{\hbar}\hat{U}^+\hat{A}_S\hat{H}\hat{U}$

$=\frac{i}{\hbar}\left(\hat{U}^+\hat{H}\hat{U}\hat{U}^+\hat{A}_S\hat{U}-\hat{U}^+\hat{A}_S\hat{U}\hat{U}^+\hat{H}\hat{U}\right)+\hat{U}^+\left(\frac{\partial\hat{A}_S}{\partial t}\right)\hat{U}$

$=\frac{i}{\hbar}[\hat{H}_H,\hat{A}_H]+\left(\frac{\partial}{\partial t}\hat{A}\right)_H$

若$\hat{H}$不显含时 $\hat{H}_H=\hat{U}^+\hat{H}_S\hat{U}=e^{i\frac{\hat{H}t}{\hbar}}\hat{H}_S e^{-i\frac{\hat{H}t}{\hbar}}=\hat{H}_S$

$\Rightarrow$ $i\hbar\frac{d}{dt}\hat{A}_H=[\hat{A}_H,\hat{H}]+i\hbar\left(\frac{\partial\hat{A}_S}{\partial t}\right)_H$ Heisenberg方程 (和经典很像)

一般这门课不显含时

例：$\hat{H}=\frac{\hat{p}^2}{2m}$

基本对易

与经典的方程只差帽子

$i\hbar\frac{d}{dt}\hat{x}=[\hat{x},\frac{\hat{p}^2}{2m}]=i\frac{\hbar}{m}\hat{p} \Rightarrow \frac{d}{dt}\hat{x}=\frac{\hat{p}}{m}$

$\Rightarrow \hat{x}(t)=\frac{\hat{p}(0)t}{m}+\hat{x}(0)$

$i\hbar\frac{d}{dt}\hat{p}=[\hat{p},\frac{\hat{p}^2}{2m}]=0 \Rightarrow \frac{d}{dt}\hat{p}=0$

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

$i\hbar\frac{d}{dt}\hat{x}=[\hat{x},\frac{\hat{p}^2}{2m}+V(\hat{x})]=\frac{i\hbar}{m}\hat{p} \Rightarrow \frac{d}{dt}\hat{x}=\frac{\hat{p}}{m}$

$i\hbar\frac{d}{dt}\hat{p}=[\hat{p},\frac{\hat{p}^2}{2m}+V(\hat{x})]=[\hat{p},V(\hat{x})]=-i\hbar\frac{\partial}{\partial\hat{x}}V(\hat{x}) \Rightarrow \frac{d\hat{p}}{dt}=-\frac{\partial V(\hat{x})}{\partial\hat{x}}$ — F (量子化牛二)

C. 相互作用绘景 (Dirac pic) 多体、微扰

态和算符都演化

$\hat{H}=\hat{H}_0+\hat{V}$ 把$\hat{H}$分成两部分去演化

定义 $|\psi(t)\rangle_I=e^{\frac{i\hat{H}_0t}{\hbar}}|\psi(t)\rangle_S$ $\hat{A}_I=e^{i\hat{H}_0t/\hbar}\hat{A}_S e^{-i\hat{H}_0t/\hbar}$

用$\hat{H}_0$往回演化t

动力学方程：
$$\begin{cases} i\hbar\frac{d}{dt}|\psi(t)\rangle_I=\hat{V}_I|\psi(t)\rangle_I, \quad \hat{V}_I=e^{i\frac{\hat{H}_0t}{\hbar}}\hat{V}_S e^{-i\frac{\hat{H}_0t}{\hbar}} \\ i\hbar\frac{d\hat{A}_I}{dt}=[\hat{A}_I,\hat{H}_0]+\left(\frac{\partial\hat{A}}{\partial t}\right)_I \end{cases}$$

时间演化方程：$i\hbar\frac{d}{dt}\hat{U}_I=\hat{V}_I\hat{U}_I \Rightarrow \hat{U}_I(t)=\hat{I}+\frac{1}{i\hbar}\int_0^t\hat{V}_I(t')U_I(t')dt'$ Dyson方程

* 三种绘景总结

SP	HP	IP
$\lvert\psi(t)\rangle_S=\lvert\psi(t)\rangle$	$\lvert\psi\rangle_H=\hat{U}^+\lvert\psi(t)\rangle_S$	$\lvert\psi\rangle_I=e^{\frac{i\hat{H}_0t}{\hbar}}\lvert\psi(t)\rangle_S$
$\hat{A}_S=\hat{A}$	$\hat{A}_H=\hat{U}^+\hat{A}_S\hat{U}$	$\hat{A}_I=e^{\frac{i\hat{H}_0t}{\hbar}}\hat{A}_S e^{-\frac{i\hat{H}_0t}{\hbar}}$
$i\hbar\frac{\partial}{\partial t}\lvert\psi(t)\rangle=\hat{H}\lvert\psi(t)\rangle$	$i\hbar\frac{d}{dt}\hat{A}_H=[\hat{A}_H,\hat{H}]+i\hbar\left(\frac{\partial\hat{A}}{\partial t}\right)_H$	$i\hbar\frac{d}{dt}\lvert\psi\rangle_I=\hat{V}_I\lvert\psi\rangle_I$; $i\hbar\frac{d}{dt}\hat{A}_I=[\hat{A}_I,\hat{H}_0]+\left(\frac{\partial\hat{A}}{\partial t}\right)_I$