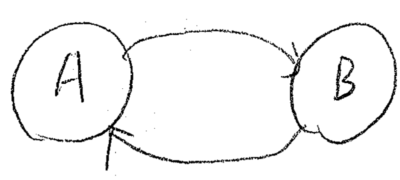
$\hat{H} = \hat{H}_0 + \hat{H}_1$

为了了解此系统

$\Downarrow$

求波函数与本征值

$\hat{H}$:



$\hat{H}_0$指单独的A、B

$\hat{H}_1$指A与B之间的相互作用

三大表象：Schrödinger (S), Heisenberg (H), Interaction (I)

表象	算符	波函数
S	不随时间演化（$\hat{H}$可以例外）	随时间演化
H	随时间演化	不随时间演化
I	随时间演化	随时间演化

S: $i\hbar \frac{\partial \psi_s(t)}{\partial t} = \hat{H}\psi_s(t)$

如果$\hat{H}$不含时，其解为

$$\psi_s(t) = e^{-iH(t-t_0)/\hbar}\psi_s(t_0)$$

注意：算符的期望值在三个表象下是不变的

即 $\langle \psi_s(t) | \hat{O}_s | \psi_s(t) \rangle$

① $= \langle \psi_H | \hat{O}_H(t) | \psi_H \rangle$

② $= \langle \psi_I(t) | \hat{O}_I(t) | \psi_I(t) \rangle$

H: $\frac{d\hat{O}_H(t)}{dt} = \frac{1}{i\hbar}[\hat{O}_H(t), \hat{H}]$ $\Leftarrow$ 运动方程

注：三个表象下的哈密顿量是一样的

如果$\hat{H}$不含时，

$$\hat{O}_H(t) = e^{iH(t-t_0)/\hbar}\hat{O}_H(t_0)e^{-iH(t-t_0)/\hbar}$$

▲ 三个表象的关系；在初始时刻t_0：

$\psi_s(t_0) = \psi_H(t_0) = \psi_I(t_0)$

ψ_s：后随t演化；ψ_H：不变；ψ_I：后随t演化

$\hat{O}_s(t_0) = \hat{O}_H(t_0) = \hat{O}_I(t_0)$

$\hat{O}_s$：不变；$\hat{O}_H$、$\hat{O}_I$：后随时间演化

下面证明式①：$\langle \psi_s(t)|\hat{O}_s|\psi_s(t)\rangle = \langle \psi_H|\hat{O}_H(t)|\psi_H\rangle$

为方面起见，在这里 $t_0=0$

证明：$\langle \psi_s(t)|\hat{O}_s(0)|\psi_s(t)\rangle = \langle \psi_s(0)|e^{iHt/\hbar}\hat{O}_s(0)e^{-iHt/\hbar}|\psi_s(0)\rangle$

$$= \langle \psi_H(0)|\hat{O}_H(t)|\psi_H(0)\rangle$$

当$\hat{H}$不含时，常采用S表象（量子力学中）和H表象（实际工作中）。

当$\hat{H}$含时，常采用I表象。

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t)$$

I表象下，$\hat{H}_0$是$\hat{H}$不含时的部分，$\hat{H}_1(t)$是含时的部分

$$\begin{cases} \psi_I(t) = e^{i\hat{H}_0(t-t_0)/\hbar}\psi_s(t) \\ \hat{O}_I(t) = e^{i\hat{H}_0(t-t_0)/\hbar}\hat{O}_I(t_0)e^{-i\hat{H}_0(t-t_0)/\hbar} \end{cases}$$

$$\begin{aligned}
i\hbar\frac{\partial\psi_I(t)}{\partial t} &= i\hbar\frac{\partial}{\partial t}\left[e^{i\hat{H}_0(t-t_0)/\hbar}e^{-i\hat{H}(t-t_0)/\hbar}\psi_s(t_0)\right] \\
&= i\left[i\hat{H}_0\psi_I(t) + e^{i\hat{H}_0(t-t_0)/\hbar}(-i\hat{H})e^{-i\hat{H}(t-t_0)/\hbar}\psi_s(t_0)\right] \\
&= i\left[i\hat{H}_0\psi_I(t) - i\hat{H}_0\psi_I(t) - ie^{i\hat{H}_0(t-t_0)/\hbar}\hat{H}_1e^{-i\hat{H}(t-t_0)/\hbar}\psi_s(t_0)\right] \\
&= e^{i\hat{H}_0(t-t_0)/\hbar}\hat{H}_1\psi_s(t) \\
&= e^{i\hat{H}_0(t-t_0)/\hbar}\hat{H}_1e^{-i\hat{H}_0(t-t_0)/\hbar}e^{i\hat{H}_0(t-t_0)/\hbar}\psi_s(t) \\
&= \hat{H}_{1I}(t)\psi_I(t)
\end{aligned}$$

$$\frac{d\hat{O}_I(t)}{dt} = \frac{1}{i\hbar}[\hat{O}_I(t), \hat{H}_0]$$

I表象和H表象的转化

$$\psi_I(t) = e^{iH_0(t-t_0)/\hbar} e^{-iH(t-t_0)/\hbar} \psi_S(t_0)$$

因为前面已提到，$\psi_S(t_0) = \psi_H(t_0)$，所以

$$\triangle \quad \psi_I(t) = \underbrace{e^{iH_0(t-t_0)/\hbar} e^{-iH(t-t_0)/\hbar}}_{S(t,t_0)} \psi_H(t_0)$$

$S(t,t_0)$ ← 称为S矩阵

$$= S(t,t_0)\psi_I(t_0)$$

$S(t,t_0)$：表征I表象下从t_0到t的演化

$$\hat{O}_I(t) = e^{i\hat{H}_0(t-t_0)/\hbar} \hat{O}_I(t_0) e^{-i\hat{H}_0(t-t_0)/\hbar}$$

$$= e^{i\hat{H}_0(t-t_0)/\hbar} \hat{O}_H(t_0) e^{-i\hat{H}_0(t-t_0)/\hbar}$$

$$= e^{i\hat{H}_0(t-t_0)/\hbar} e^{-i\hat{H}(t-t_0)/\hbar} [e^{i\hat{H}(t-t_0)/\hbar} \hat{O}_H(t_0) e^{-i\hat{H}(t-t_0)/\hbar}] e^{i\hat{H}(t-t_0)/\hbar} e^{-i\hat{H}_0(t-t_0)/\hbar}$$

$$\triangle \quad \hat{O}_I(t) = S(t,t_0)\hat{O}_H(t) S^{\dagger}(t,t_0)$$

由 $i\hbar\frac{\partial\psi_I(t)}{\partial t} = H_{1I}(t)\psi_I(t)$ 可得

$$\psi_I(t) = \psi_I(t_0) + \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} dt' H_{1I}(t')\psi_I(t_0) + \cdots + \left(-\frac{i}{\hbar}\right)^N \int_{t_0}^{t} dt_1 H_{1I}(t_1)$$

$$\times \int_{t_0}^{t_1} dt_2 H_{1I}(t_2) \cdots \int_{t_0}^{t_{n-1}} dt_n H_{1I}(t_n)\psi_I(t_0) \qquad n = \infty$$

$$= S(t,t_0)\psi_I(t_0)$$

前面我们提到

$$S(t,t_0)=e^{iH_0(t-t_0)/\hbar}e^{-iH(t-t_0)/\hbar} \quad ③$$

而在此处

$$S(t,t_0)=1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}dt' H_{1I}(t')+\cdots+\left(-\frac{i}{\hbar}\right)^N\int_{t_0}^{t}dt_1 H_{1I}(t_1)$$
$$\times\int_{t_0}^{t}dt_2 H_{1I}(t_2)\cdots\int_{t_0}^{t_{n-1}}dt_n H_{1I}(t_n) \qquad n=\infty \quad ④$$

两者是等价的，证明：③满足方程

$$\frac{\partial}{\partial t}S(t,t_0)=\frac{i}{\hbar}H_0 e^{iH_0(t-t_0)/\hbar}e^{-iH(t-t_0)/\hbar}$$
$$+e^{iH_0(t-t_0)/\hbar}\left(\frac{-i}{\hbar}H\right)e^{-iH(t-t_0)/\hbar}$$
$$=e^{iH_0(t-t_0)/\hbar}\left(\frac{-i}{\hbar}H_1\right)e^{-iH(t-t_0)/\hbar}$$
$$=\frac{-i}{\hbar}\left[e^{iH_0(t-t_0)/\hbar}H_1e^{-iH_0(t-t_0)/\hbar}\right]e^{iH_0(t-t_0)/\hbar}e^{-iH(t-t_0)/\hbar}$$
$$=\frac{-i}{\hbar}H_{1I}(t)S(t,t_0)$$

方程两边对时间积分，得

左边：$\int_{t_0}^{t}dt_1\frac{\partial}{\partial t_1}S(t_1,t_0)=S(t,t_0)-S(t_0,t_0)$

右边：$-\frac{i}{\hbar}\int_{t_0}^{t}dt_1 H_{1I}(t_1)S(t_1,t_0)$

注：$S(t_0,t_0)=1$ 结合起来，有

$$S(t,t_0)=1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}dt_1 H_{1I}(t_1)S(t_1,t_0)$$

展开

$$S(t,t_0)=1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}dt_1 H_{1I}(t_1)+\left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}dt_1 H_{1I}(t_1)\int_{t_0}^{t_1}dt_2 H_{1I}(t_2)$$

$$+\cdots+\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1 H_{1I}(t_1)\cdots\int_{t_0}^{t_{n-1}}dt_n H_{1I}(t_n) \qquad n=\infty$$

证毕

上式可进一步写为

作业6. 证明此关系成立

$$S(t,t_0)=\hat{T}\exp\left\{\frac{-i}{\hbar}\int_{t_0}^{t}H_{1I}(t')dt'\right\}$$

$\hat{T}$ 为编时算符

$$\hat{T}[a(t_1)\,a(t_2)]=\begin{cases}a(t_1)\,a(t_2) & t_1>t_2\\ \mp\, a(t_2)\,a(t_1) & t_2>t_1\end{cases}$$

$-$ 表示费米子，$+$ 表示玻色子

总结 $S(t,t_0)$ 的性质

① $t=t_0$，$S(t,t_0)=1$

② $S(t_2,t_0)=S(t_2,t_1)\,S(t_1,t_0)$ 作业7

③ 多体物理中，绝热引入相互作用，$t_0\to-\infty$ 时，$H'\to 0$

④ $t_0\to-\infty$，$e^{iHt/\hbar}=S^{-1}(t,-\infty)\,e^{iH_0t/\hbar}$ 作业7

作业 6

证明：$S(t,t_0)=\hat{T}\exp\{\frac{-i}{\hbar}\int_{t_0}^{t}H_{1I}(t')\,dt'\}$

$$S(t,t_0)=1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}dt_1H_{1I}(t_1)+\cdots+\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1H_{1I}(t_1)\cdots\int_{t_0}^{t_{n-1}}dt_nH_{1I}(t_n)$$

$$=1+\sum_{j=1}^{\infty}\left(\frac{-i}{\hbar}\right)^j\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{j-1}}dt_j\,H_{1I}(t_1)H_{1I}(t_2)\cdots H_{1I}(t_j)\quad ②$$

$$=1+\sum_{j=1}^{\infty}\frac{1}{j!}\left(\frac{-i}{\hbar}\right)^j\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\cdots\int_{t_0}^{t}dt_j\,H_{1I}(t_1)H_{1I}(t_2)\cdots H_{1I}(t_j)\quad ③$$

通过数学归纳法可证明 ② = ③

首先 当 $j=1$时，② : $1+\frac{-i}{\hbar}\int_{t_0}^{t}dt_1H_{1I}(t_1)$

③ : $1+\frac{-i}{\hbar}\int_{t_0}^{t}dt_1H_{1I}(t_1)$

② = ③ ，命题成立。

假设 $j=n$时，② = ③.

现在证明当 $j=n+1$ 时，② = ③

$j=n$时，$②_n$: $1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}dt_1H_{1I}(t_1)+\cdots+\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1H_{1I}(t_1)\cdots\int_{t_0}^{t_{n-1}}dt_nH_{1I}(t$

$③_n$: $1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}dt_1H_{1I}(t_1)+\cdots+\left(\frac{1}{n!}\right)\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_n\,H_{1I}(t_1)\cdots H_{1I}($

根据假设，$②_n=③_n$

当 $j=n+1$时，

$$②_{n+1}=②_n+\underbrace{\left(\frac{-i}{\hbar}\right)^{n+1}\int_{t_0}^{t}dt_1H_{1I}(t_1)\cdots\int_{t_0}^{t_{n-1}}dt_nH_{1I}(t_n)\int_{t_0}^{t_n}dt_{n+1}\,H_{1I}(t_{n+1})}$$

$$=③_n+[\qquad\qquad]$$

如果设 $\frac{\partial F(t)}{\partial t} = H_{1I}(t)$，那么

$$\int_{t_0}^{t_n} dt_{n+1} H_{1I}(t_{n+1}) = F(t_n) - F(t_0)$$

$$\int_{t_0}^{t_{n-1}} dt_n H_{1I}(t_n) \int_{t_0}^{t_n} dt_{n+1} H_{1I}(t_{n+1}) = \int_{t_0}^{t_{n-1}} [F(t_n) - F(t_0)] \frac{\partial F(t_n)}{\partial t_n} dt_n$$

$$= \int_{t_0}^{t_{n-1}} \frac{\partial F(t_n)}{\partial t_n} F(t_n) - \frac{\partial F(t_n)}{\partial t_n} F(t_0)\, dt_n$$

$$= \frac{1}{2} F^2(t_n) \Big|_{t_0}^{t_{n-1}} - F(t_0) F(t_n) \Big|_{t_0}^{t_{n-1}}$$

$$= \frac{1}{2}[F^2(t_{n-1}) - F^2(t_0)] - F(t_0) F(t_{n-1}) + F^2(t_0)$$

$$= \frac{1}{2}[F^2(t_{n-1}) + F^2(t_0)] - F(t_0) F(t_{n-1}) = \frac{1}{2}[F(t_{n-1}) - F(t_0)]^2$$

$$\int_{t_0}^{t_{n-2}} dt_{n-1} H_{1I}(t_{n-1}) \int_{t_0}^{t_{n-1}} dt_n H_{1I}(t_n) \int_{t_0}^{t_n} dt_{n+1} H_{1I}(t_{n+1})$$

$$= \int_{t_0}^{t_{n-2}} dt_{n-1} \frac{\partial F(t_{n-1})}{\partial t_{n-1}} \frac{1}{2}[F(t_{n-1}) - F(t_0)]^2$$

$$= F(t_{n-1}) \frac{1}{2}[F(t_{n-1}) - F(t_0)]^2 \Big|_{t_0}^{t_{n-2}} - \int_{t_0}^{t_{n-2}} dt_{n-1} [F(t_{n-1}) - F(t_0)] F(t_{n-1}) \frac{\partial F(t_{n-1})}{\partial t_{n-1}}$$

$$= \frac{1}{2} F(t_{n-2}) [F(t_{n-2}) - F(t_0)]^2 - \frac{1}{3} F^3(t_{n-1}) \Big|_{t_0}^{t_{n-2}} + \frac{1}{2} F(t_0) F^2(t_{n-1}) \Big|_{t_0}^{t_{n-2}}$$

$$= \frac{1}{6} F^3(t_{n-2}) + \frac{1}{2} F^2(t_0) F(t_{n-2}) - \frac{1}{2} F(t_0) F^2(t_{n-2}) - \frac{1}{6} F^3(t_0)$$

$$= \frac{1}{6} [F(t_{n-2}) - F(t_0)]^3$$

由此递推，可得

$$\left[\int_{t_0}^{t} dt_1 H_{1I}(t_1) \int_{t_0}^{t_1} dt_2 H_{1I}(t_2) \cdots \int_{t_0}^{t_n} dt_{n+1} H_{1I}(t_n)\right] \left(\frac{-i}{\hbar}\right)^{n+1}$$

$$= \frac{1}{(n+1)!} [F(t) - F(t_0)]^{n+1} \left(\frac{-i}{\hbar}\right)^{n+1}$$

$$= \frac{1}{(n+1)!} \left(\frac{-i}{\hbar}\right)^{n+1} \int_{t_0}^{t} dt_1 H_{1I}(t_1) \int_{t_0}^{t} dt_2 H_{1I}(t_2) \cdots \int_{t_0}^{t} dt_{n+1} H_{1I}(t_{n+1})$$

现在回到 $j=n+1$ 时的证明

$$②_{n+1} = ③_n + \frac{1}{(n+1)!}\left(\frac{-i}{\hbar}\right)^{n+1}\int_{t_0}^{t} dt_1 H_{1I}(t_1)\int_{t_0}^{t} dt_2 H_{1I}(t_2)\cdots\int_{t_0}^{t} dt_{n+1} H_{1I}(t_{n+1})$$

$$= ③_{n+1}$$

因此 ② = ③ ，证毕

进一步在 ③ 的基础上推导 $S(t,t_0)$

$$S(t,t_0) = 1 + \sum_{j=1}^{\infty}\frac{1}{j!}\left(\frac{-i}{\hbar}\right)^{j}\int_{t_0}^{t} dt_1\int_{t_0}^{t} dt_2\cdots\int_{t_0}^{t} dt_j H_{1I}(t_1)H_{1I}(t_2)\cdots H_{1I}(t_j)$$

$$= \hat{T}\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} H_{1I}(t_1)dt_1\right\}$$

Talor展开

作业6 证毕　　$\hat{T}$的作用是保证 $t_0 \le t$

作业7.1 证明 $S(t_2,t_0) = S(t_2,t_1)S(t_1,t_0)$

因为 $t_0 \le t_1 \le t_2$ ，所以省略 $\hat{T}$

$$S(t_2,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t_2} H_{1I}(t')dt'}$$

$$S(t_2,t_1) = e^{-\frac{i}{\hbar}\int_{t_1}^{t_2} H_{1I}(t')dt'}$$

$$S(t_1,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t_1} H_{1I}(t')dt'}$$

$$S(t_2,t_1)S(t_1,t_0) = e^{-\frac{i}{\hbar}\left[\int_{t_1}^{t_2} H_{1I}(t')dt' + \int_{t_0}^{t_1} H_{1I}(t')dt'\right]}$$

$$= e^{-\frac{i}{\hbar}\int_{t_0}^{t_2} H_{1I}(t')dt'}$$

$$= S(t_2,t_0)$$

证毕

作业 7.2 证明 $t_0 \to -\infty$ 时, $e^{iHt/\hbar} = S^{-1}(t,-\infty)e^{iH_0t/\hbar}$

在正文中, 我们已证明 $S(t,t_0)$ 可写为

$$S(t,t_0) = e^{iH_0(t-t_0)/\hbar} e^{-iH(t-t_0)/\hbar}$$

因此 $S(t,t_0)e^{iHt} = e^{iH_0t/\hbar} e^{i(H-H_0)t_0/\hbar}$

当 $t_0 \to -\infty$ 时, $H_1 \to 0$ (因为假设了 $t_0 \to \infty$ 时, 系统没有相互作用)

所以 $S(t,-\infty)e^{iHt} = e^{iH_0t/\hbar}$

$$e^{iHt} = S^{-1}(t,-\infty)e^{iH_0t/\hbar}$$

证毕