# 课堂练习

## 练习1：证明概率流通量具有如下性质：$\int d^3x\boldsymbol{j}(\boldsymbol{x},t)=\frac{\langle\hat{\boldsymbol{p}}\rangle(t)}{m}$

**证明**：根据埃伦费斯特定理，有$\frac{d}{dt}\langle\hat{\boldsymbol{x}}\rangle(t)=\frac{\langle\hat{\boldsymbol{p}}\rangle(t)}{m}$，又知

$$\langle\hat{\boldsymbol{x}}\rangle(t)=\int\psi(\boldsymbol{x},t)^*\hat{\boldsymbol{x}}\psi(\boldsymbol{x},t)d^3x=\int\boldsymbol{x}\psi(\boldsymbol{x},t)^*\psi(\boldsymbol{x},t)d^3x$$

因此对时间求导得

$$\frac{d}{dt}\langle\hat{\boldsymbol{x}}\rangle(t)=\int\boldsymbol{x}[\frac{\partial\psi(\boldsymbol{x},t)^*}{\partial t}\psi(\boldsymbol{x},t)+\psi(\boldsymbol{x},t)^*\frac{\psi(\boldsymbol{x},t)}{\partial t}]d^3x$$

又知含时薛定谔方程为$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)=\hat{H}\psi(\boldsymbol{x},t)$，取复共轭得$-\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)^*=\hat{H}\psi(\boldsymbol{x},t)^*$，而哈密尔顿算符可写成$\hat{H}=-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2+V(\hat{\boldsymbol{x}})$，其中$V(\hat{\boldsymbol{x}})$为关于算符$\hat{\boldsymbol{x}}$的实函数，因此有
$\begin{cases}\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)=-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)+V(\hat{\boldsymbol{x}})\psi(\boldsymbol{x},t)\\-\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)^*=-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)^*+V(\hat{\boldsymbol{x}})\psi(\boldsymbol{x},t)^*\end{cases}$，从而

$$\begin{aligned}&\frac{\partial\psi(\boldsymbol{x},t)^*}{\partial t}\psi(\boldsymbol{x},t)+\psi(\boldsymbol{x},t)^*\frac{\psi(\boldsymbol{x},t)}{\partial t}\\=&-\frac{1}{\mathrm{i}\hbar}[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)^*+V(\hat{\boldsymbol{x}})\psi(\boldsymbol{x},t)^*]\cdot\psi(\boldsymbol{x},t)+\psi(\boldsymbol{x},t)^*\cdot\frac{1}{\mathrm{i}\hbar}[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)+V(\hat{\boldsymbol{x}})\psi(\boldsymbol{x},t)]\\=&-\frac{1}{\mathrm{i}\hbar}[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)^*+V(\boldsymbol{x})\psi(\boldsymbol{x},t)^*]\cdot\psi(\boldsymbol{x},t)+\psi(\boldsymbol{x},t)^*\cdot\frac{1}{\mathrm{i}\hbar}[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)+V(\boldsymbol{x})\psi(\boldsymbol{x},t)]\\=&\frac{\mathrm{i}\hbar}{2m}[-\psi(\boldsymbol{x},t)\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)^*+\psi(\boldsymbol{x},t)^*\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)]\\=&\frac{\mathrm{i}\hbar}{2m}[-\psi(\boldsymbol{x},t)\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)^*-\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)^*+\psi(\boldsymbol{x},t)^*\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x},t)+\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)^*]\\=&\frac{\mathrm{i}\hbar}{2m}\nabla_{\boldsymbol{x}}\cdot[-\psi(\boldsymbol{x},t)\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)^*+\psi(\boldsymbol{x},t)^*\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)]\end{aligned}$$

记概率通量为

$$\boldsymbol{j}(\boldsymbol{x},t)=-\frac{\mathrm{i}\hbar}{2m}[\psi(\boldsymbol{x},t)^*\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)-\psi(\boldsymbol{x},t)\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)^*]$$

则（此处用到边界条件）

$$\frac{d}{dt}\langle\hat{\boldsymbol{x}}\rangle(t)=\int_V\boldsymbol{x}[-\nabla_{\boldsymbol{x}}\cdot\boldsymbol{j}(\boldsymbol{x},t)]d^3x=[-\boldsymbol{x}\boldsymbol{j}(\boldsymbol{x},t)]_V-\int_V(\nabla_{\boldsymbol{x}}\boldsymbol{x})\cdot[-\boldsymbol{j}(\boldsymbol{x},t)]d^3x=\int_V\boldsymbol{j}(\boldsymbol{x},t)d^3x$$

故最终$\int d^3x\boldsymbol{j}(\boldsymbol{x},t)=\frac{\langle\hat{\boldsymbol{p}}\rangle(t)}{m}$

## 练习2：推导$\frac{d\hat{O}_I(t)}{dt}=\frac{1}{\mathrm{i}\hbar}[\hat{O}_I(t),\hat{H}_0]$

**解**：由于$\hat{O}_I(t)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{O}_I(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0t}$，因此对时间求导得

$$\begin{aligned}\frac{d\hat{O}_I(t)}{dt}&=\frac{d[\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{O}_I(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0t}]}{dt}=\frac{\mathrm{i}}{\hbar}[\hat{H}_0\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{O}_I(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0t}-\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{O}_I(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{H}_0]\\&=\frac{\mathrm{i}}{\hbar}[\hat{H}_0\hat{O}_I(t)-\hat{O}_I(t)\hat{H}_0]=\frac{1}{\mathrm{i}\hbar}[\hat{O}_I(t),\hat{H}_0]\end{aligned}$$

## 练习3：写出相互作用表象和薛定谔表象下时间演化算符之间的关系

**解**：设$t_0$时刻两种表象的态矢重合，即$|\alpha(t_0)\rangle_I = |\alpha(t_0)\rangle_S$，则$t$时刻，两种表象的态矢满足$|\alpha(t)\rangle_I = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0(t-t_0)}|\alpha(t)\rangle_S$，记$\hat{U}^\dagger_{\hat{H}_0}(t,t_0) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0(t-t_0)}$，则$|\alpha(t)\rangle_I = \hat{U}^\dagger_{\hat{H}_0}(t,t_0)|\alpha(t)\rangle_S = \hat{U}^\dagger_{\hat{H}_0}(t,t_0)\hat{U}(t,t_0)|\alpha(t_0)\rangle_S$，又$|\alpha(t)\rangle_I = \hat{U}_I(t,t_0)|\alpha(t_0)\rangle_I$，因此$\hat{U}_I(t,t_0) = \hat{U}^\dagger_{\hat{H}_0}(t,t_0)\hat{U}(t,t_0)$

## 练习4：精确求解含时两能级问题，其中零级哈密尔顿算符$\hat{H}_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$，微扰项$\hat{H}' = \gamma\mathrm{e}^{\mathrm{i}\omega t}|1\rangle\langle 2| + \gamma\mathrm{e}^{-\mathrm{i}\omega t}|2\rangle\langle 1|$

**解**：该体系的运动方程为$\mathrm{i}\hbar\begin{pmatrix}\dot{c}_1(t)\\ \dot{c}_2(t)\end{pmatrix} = \begin{pmatrix}0 & \gamma\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}\omega_{12}t}\\ \gamma\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}\omega_{21}t} & 0\end{pmatrix}\begin{pmatrix}c_1(t)\\ c_2(t)\end{pmatrix}$，其中$\omega_{21} = -\omega_{12} = \frac{E_2-E_1}{\hbar}$，化成方程组形式，我们有$\begin{cases}\mathrm{i}\hbar\frac{\partial c_1(t)}{\partial t} = \gamma\mathrm{e}^{\mathrm{i}(\omega-\omega_{21})t}c_2(t)\\ \mathrm{i}\hbar\frac{\partial c_2(t)}{\partial t} = \gamma\mathrm{e}^{-\mathrm{i}(\omega-\omega_{21})t}c_1(t)\end{cases}$，将该方程组对时间求导，得

$$\begin{cases}\mathrm{i}\hbar\frac{\partial^2 c_1(t)}{\partial t^2} = \mathrm{i}(\omega-\omega_{21})\gamma\mathrm{e}^{\mathrm{i}(\omega-\omega_{21})t}c_2(t) + \gamma\mathrm{e}^{\mathrm{i}(\omega-\omega_{21})t}\frac{\partial c_2(t)}{\partial t}\\ \mathrm{i}\hbar\frac{\partial^2 c_2(t)}{\partial t^2} = -\mathrm{i}(\omega-\omega_{21})\gamma\mathrm{e}^{-\mathrm{i}(\omega-\omega_{21})t}c_1(t) + \gamma\mathrm{e}^{-\mathrm{i}(\omega-\omega_{21})t}\frac{\partial c_1(t)}{\partial t}\end{cases}$$

两个方程组联立，经化简得

$$\begin{cases}\mathrm{i}\hbar\frac{\partial^2 c_1(t)}{\partial t^2} = \mathrm{i}(\omega-\omega_{21})\cdot\mathrm{i}\hbar\frac{\partial c_1(t)}{\partial t} + \gamma\mathrm{e}^{\mathrm{i}(\omega-\omega_{21})t}\cdot\frac{\gamma\mathrm{e}^{-\mathrm{i}(\omega-\omega_{21})t}c_1(t)}{\mathrm{i}\hbar}\\ \mathrm{i}\hbar\frac{\partial^2 c_2(t)}{\partial t^2} = -\mathrm{i}(\omega-\omega_{21})\cdot\mathrm{i}\hbar\frac{\partial c_2(t)}{\partial t} + \gamma\mathrm{e}^{-\mathrm{i}(\omega-\omega_{21})t}\cdot\frac{\gamma\mathrm{e}^{\mathrm{i}(\omega-\omega_{21})t}c_2(t)}{\mathrm{i}\hbar}\end{cases} \Rightarrow \begin{cases}\frac{\partial^2 c_1(t)}{\partial t^2} - \mathrm{i}(\omega-\omega_{21})\frac{\partial c_1(t)}{\partial t} + \frac{\gamma^2}{\hbar^2}c_1(t) = 0\\ \frac{\partial^2 c_2(t)}{\partial t^2} + \mathrm{i}(\omega-\omega_{21})\frac{\partial c_2(t)}{\partial t} + \frac{\gamma^2}{\hbar^2}c_2(t) = 0\end{cases}$$

相应的特征方程为$\begin{cases}r^2 - \mathrm{i}(\omega-\omega_{21})r + \frac{\gamma^2}{\hbar^2} = 0\\ s^2 + \mathrm{i}(\omega-\omega_{21})s + \frac{\gamma^2}{\hbar^2} = 0\end{cases}$，即$\begin{cases}r = \frac{\mathrm{i}(\omega-\omega_{21})\pm\mathrm{i}\sqrt{(\omega-\omega_{21})^2+\frac{4\gamma^2}{\hbar^2}}}{2}\\ s = \frac{-\mathrm{i}(\omega-\omega_{21})\pm\mathrm{i}\sqrt{(\omega-\omega_{21})^2+\frac{4\gamma^2}{\hbar^2}}}{2}\end{cases}$，因此原微分方程的通解为（记$\Omega = \sqrt{(\omega-\omega_{21})^2+\frac{4\gamma^2}{\hbar^2}}$）：

$$\begin{cases}c_1(t) = \mathrm{e}^{\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(A\cos\frac{\Omega t}{2} + B\sin\frac{\Omega t}{2})\\ c_2(t) = \mathrm{e}^{-\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(C\cos\frac{\Omega t}{2} + D\sin\frac{\Omega t}{2})\end{cases}$$

相应的导数为

$$\begin{cases}\frac{\partial c_1(t)}{\partial t} = \frac{\mathrm{i}(\omega-\omega_{21})}{2}\mathrm{e}^{\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(A\cos\frac{\Omega t}{2} + B\sin\frac{\Omega t}{2}) + \frac{\Omega}{2}\mathrm{e}^{\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(-A\sin\frac{\Omega t}{2} + B\cos\frac{\Omega t}{2})\\ \frac{\partial c_2(t)}{\partial t} = -\frac{\mathrm{i}(\omega-\omega_{21})}{2}\mathrm{e}^{-\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(C\cos\frac{\Omega t}{2} + D\sin\frac{\Omega t}{2}) + \frac{\Omega}{2}\mathrm{e}^{-\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(-C\sin\frac{\Omega t}{2} + D\cos\frac{\Omega t}{2})\end{cases}$$

假设初始状态（$t=0$）下，体系处于状态$|1\rangle$，即$c_1(0)=1$，$c_2(0)=0$，则

$$\begin{cases}c_1(0) = A = 1\\ c_2(0) = C = 0\\ \mathrm{i}\hbar\dot{c}_1(0) = \mathrm{i}\hbar[\frac{\mathrm{i}(\omega-\omega_{21})}{2}A + \frac{\Omega}{2}B] = \gamma c_2(0) = 0\\ \mathrm{i}\hbar\dot{c}_2(0) = \mathrm{i}\hbar[-\frac{\mathrm{i}(\omega-\omega_{21})}{2}C + \frac{\Omega}{2}D] = \gamma c_1(0) = \gamma\end{cases} \Rightarrow \begin{cases}A = 1\\ B = -\frac{\mathrm{i}(\omega-\omega_{21})}{\Omega}\\ C = 0\\ D = \frac{2\gamma}{\mathrm{i}\hbar\Omega}\end{cases}$$

因此符合初始条件的原微分方程的解为（记$\Omega_0 = \frac{2\gamma}{\hbar}$）$\begin{cases}c_1(t) = \mathrm{e}^{\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(\cos\frac{\Omega t}{2} - \frac{\omega-\omega_{21}}{\Omega}\mathrm{i}\sin\frac{\Omega t}{2})\\ c_2(t) = \mathrm{e}^{-\frac{\mathrm{i}(\omega-\omega_{21})t}{2}}(-\frac{\Omega_0}{\Omega}\mathrm{i}\sin\frac{\Omega t}{2})\end{cases}$，

而模的平方为$\begin{cases}|c_1(t)|^2 = \cos^2\frac{\Omega t}{2} + \frac{\Omega^2-\Omega_0^2}{\Omega^2}\sin^2\frac{\Omega t}{2} = 1 - |c_1(t)|^2\\ |c_2(t)|^2 = \frac{\Omega_0^2}{\Omega^2}\sin^2\frac{\Omega t}{2}\end{cases}$

### 练习5：对含时常微扰问题考虑二阶修正，推导出$c_n^{(2)}(\tau)$的计算表达式，讨论$\tau$足够大时的平均跃迁速率

**解**：考虑二阶修正，则有（记$\omega_{nm}=\frac{E_n-E_m}{\hbar}$，$\omega_{mi}=\frac{E_m-E_i}{\hbar}$，$\omega_{ni}=\omega_{nm}+\omega_{mi}=\frac{E_n-E_i}{\hbar}$）：

$$
\begin{aligned}
c_n^{(2)}(\tau)&=(-\frac{\mathrm{i}}{\hbar})^2\int_0^\tau dt_1\int_0^{t_1}dt_2\langle n|\hat{H}_I^{'}(t_1)\hat{H}_I^{'}(t_2)|i\rangle=(-\frac{\mathrm{i}}{\hbar})^2\sum_m\int_0^\tau dt_1\int_0^{t_1}dt_2\langle n|\hat{H}_I^{'}(t_1)|m\rangle\langle m|\hat{H}_I^{'}(t_2)|i\rangle\\
&=-\frac{1}{\hbar^2}\sum_m\int_0^\tau dt_1\int_0^{t_1}dt_2\mathrm{e}^{\mathrm{i}\omega_{nm}t_1}V_{nm}\mathrm{e}^{\mathrm{i}\omega_{mi}t_2}V_{mi}=-\sum_m\frac{V_{nm}V_{mi}}{\hbar^2}\int_0^\tau\mathrm{e}^{\mathrm{i}\omega_{nm}t_1}dt_1\int_0^{t_1}\mathrm{e}^{\mathrm{i}\omega_{mi}t_2}dt_2\\
&=-\sum_m\frac{V_{nm}V_{mi}}{\hbar^2}\int_0^\tau\mathrm{e}^{\mathrm{i}\omega_{nm}t_1}dt_1\cdot(\frac{\mathrm{e}^{\mathrm{i}\omega_{mi}t_1}-1}{\mathrm{i}\omega_{mi}})=-\sum_m\frac{V_{nm}V_{mi}}{\mathrm{i}\hbar^2\omega_{mi}}\int_0^\tau[\mathrm{e}^{\mathrm{i}(\omega_{nm}+\omega_{mi})t_1}-\mathrm{e}^{\mathrm{i}\omega_{nm}t_1}]dt_1\\
&=-\sum_m\frac{V_{nm}V_{mi}}{\mathrm{i}\hbar^2\omega_{mi}}[\frac{\mathrm{e}^{\mathrm{i}(\omega_{nm}+\omega_{mi})\tau}-1}{\mathrm{i}(\omega_{nm}+\omega_{mi})}-\frac{\mathrm{e}^{\mathrm{i}\omega_{nm}\tau}-1}{\mathrm{i}\omega_{nm}}]=-\sum_m\frac{V_{nm}V_{mi}}{\mathrm{i}\hbar^2\omega_{mi}}[\frac{\mathrm{e}^{\mathrm{i}\omega_{ni}\tau}-1}{\mathrm{i}\omega_{ni}}-\frac{\mathrm{e}^{\mathrm{i}\omega_{nm}\tau}-1}{\mathrm{i}\omega_{nm}}]\\
&=-\sum_m\frac{V_{nm}V_{mi}}{\mathrm{i}\hbar^2\omega_{mi}}[\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}\frac{\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}-\mathrm{e}^{-\frac{\mathrm{i}\omega_{ni}\tau}{2}}}{\mathrm{i}\omega_{ni}}-\mathrm{e}^{\frac{\mathrm{i}\omega_{nm}\tau}{2}}\frac{\mathrm{e}^{\frac{\mathrm{i}\omega_{nm}\tau}{2}}-\mathrm{e}^{-\frac{\mathrm{i}\omega_{nm}\tau}{2}}}{\mathrm{i}\omega_{nm}}]\\
&=\sum_m\frac{\mathrm{i}V_{nm}V_{mi}}{\hbar^2\omega_{mi}}[\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}}-\mathrm{e}^{\frac{\mathrm{i}\omega_{nm}\tau}{2}}\frac{\sin\frac{\omega_{nm}\tau}{2}}{\frac{\omega_{nm}}{2}}]
\end{aligned}
$$

结合一阶修正$c_n^{(1)}(\tau)=-\frac{\mathrm{i}V_{ni}}{\hbar}\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}}$，得跃迁概率（未完待续）

$$
\begin{aligned}
P_{i\to n}^{(2)}(\tau)=|c_n^{(1)}(\tau)+c_n^{(2)}(\tau)|^2&=\Big|-\frac{\mathrm{i}V_{ni}}{\hbar}\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}}+\sum_m\frac{\mathrm{i}V_{nm}V_{mi}}{\hbar^2\omega_{mi}}[\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}}-\mathrm{e}^{\frac{\mathrm{i}\omega_{nm}\tau}{2}}\frac{\sin\frac{\omega_{nm}\tau}{2}}{\frac{\omega_{nm}}{2}}]\Big|^2\\
&=\Big|(-\frac{\mathrm{i}V_{ni}}{\hbar}+\sum_m\frac{\mathrm{i}V_{nm}V_{mi}}{\hbar^2\omega_{mi}})\mathrm{e}^{\frac{\mathrm{i}\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}}-\sum_m\frac{\mathrm{i}V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\mathrm{e}^{\frac{\mathrm{i}\omega_{nm}\tau}{2}}\frac{\sin\frac{\omega_{nm}\tau}{2}}{\frac{\omega_{nm}}{2}}\Big|^2\\
&=\Big|-\frac{V_{ni}}{\hbar}+\sum_m\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\frac{\sin^2\frac{\omega_{ni}\tau}{2}}{(\frac{\omega_{ni}}{2})^2}+\sum_m\Big|\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\frac{\sin^2\frac{\omega_{nm}\tau}{2}}{(\frac{\omega_{nm}}{2})^2}+\text{交叉项}
\end{aligned}
$$

利用$\delta$函数的定义$\lim\limits_{a \rightarrow \infty} \frac{\sin^2(ax)}{\pi ax^2}=\delta(x)$，我们有

$$
\frac{\sin^2\frac{\omega_{ni}\tau}{2}}{(\frac{\omega_{ni}}{2})^2}=\pi\tau\delta(\frac{\omega_{ni}}{2})=2\pi\tau\delta(\omega_{ni})\quad\frac{\sin^2\frac{\omega_{nm}\tau}{2}}{(\frac{\omega_{nm}}{2})^2}=\pi\tau\delta(\frac{\omega_{nm}}{2})=2\pi\tau\delta(\omega_{nm})
$$

由于交叉项包含两项交叉乘积，来自干涉的贡献，可以忽略，因此我们有

$$
P_{i\to n}^{(2)}(\tau)\approx2\pi\tau\Big[\Big|-\frac{V_{ni}}{\hbar}+\sum_m\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\delta(\omega_{ni})+\sum_m\Big|\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\delta(\omega_{nm})\Big]
$$

$$
w_{i\to n}^{(2)}=\frac{P_{i\to n}^{(2)}(\tau)}{\tau}=2\pi\Big[\Big|-\frac{V_{ni}}{\hbar}+\sum_m\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\delta(\omega_{ni})+\sum_m\Big|\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\delta(\omega_{nm})\Big]\approx2\pi\Big|-\frac{V_{ni}}{\hbar}+\sum_m\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2\delta(\omega_{ni})
$$

### 练习6：证明$\hat{Q}_n^2=\hat{Q}_n$，其中$\hat{Q}_n=\hat{I}-| n^{(0)} \rangle \langle n^{(0)} |=\sum\limits_{k \neq n} | k^{(0)} \rangle \langle k^{(0)} |$

**证明**：（方法1）设$\hat{P}_n \equiv | n^{(0)} \rangle \langle n^{(0)} |$，则$\hat{P}_n^2=| n^{(0)} \rangle \langle n^{(0)} | n^{(0)} \rangle \langle n^{(0)} |=| n^{(0)} \rangle \langle n^{(0)} |=\hat{P}_n$，因此

$$
\hat{Q}_n^2=(\hat{I}-\hat{P}_n)^2=\hat{I}-2\hat{P}_n+\hat{P}_n^2=\hat{I}-2\hat{P}_n+\hat{P}_n=\hat{I}-\hat{P}_n=\hat{Q}_n
$$

（方法2）显然

$$\hat{Q}_n^2=\sum_{k\neq n}|k^{(0)}\rangle\langle k^{(0)}|\sum_{l\neq n}|l^{(0)}\rangle\langle l^{(0)}|=\sum_{k\neq n,l\neq n}|k^{(0)}\rangle\langle k^{(0)}|l^{(0)}\rangle\langle l^{(0)}|=\sum_{k\neq n,l\neq n}\delta_{kl}|k^{(0)}\rangle\langle l^{(0)}|=\sum_{k\neq n}|k^{(0)}\rangle\langle k^{(0)}|=\hat{Q}_n$$

# 第五章习题

## 5.1 设$t=0$时，电子处于$\hat{S}_x$的本征态$| s_x+ \rangle$，用海森堡表象求解电子在恒定$z$方向磁场$B$中的进动$\hat{H}=-(\frac{eB}{mc})\hat{S}_z=\omega \hat{S}_z$，获得$\langle \hat{S}_x \rangle$，$\langle \hat{S}_y \rangle$，$\langle \hat{S}_z \rangle$随时间的变化

**解**：海森堡表象下，态矢为$| u \rangle=| s_x+ \rangle=\frac{1}{\sqrt{2}}(| s_z+ \rangle+| s_z- \rangle)$，而算符随时间演化变为：

$$\begin{aligned}\hat{S}_x(t)=\hat{U}^\dagger(t)\hat{S}_x(0)\hat{U}(t)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{S}_x(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=\mathrm{e}^{\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_x(0)\mathrm{e}^{-\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\\ \hat{S}_y(t)=\hat{U}^\dagger(t)\hat{S}_y(0)\hat{U}(t)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{S}_y(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=\mathrm{e}^{\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_y(0)\mathrm{e}^{-\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\\ \hat{S}_z(t)=\hat{U}^\dagger(t)\hat{S}_z(0)\hat{U}(t)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{S}_z(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=\mathrm{e}^{\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_z(0)\mathrm{e}^{-\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}=\hat{S}_z(0)\end{aligned}$$

因此t时刻各个自旋算符的期望值为

$$\begin{aligned}\langle\hat{S}_x\rangle(t)&=\langle u|\hat{S}_x(t)|u\rangle=[\frac{1}{\sqrt{2}}(\langle s_z+|+\langle s_z-|)]\mathrm{e}^{\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_x(0)\mathrm{e}^{-\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}[\frac{1}{\sqrt{2}}(|s_z+\rangle+|s_z-\rangle)]\\ &=\frac{1}{2}(\langle s_z+|\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}+\langle s_z-|\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}})\hat{S}_x(0)(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|s_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|s_z-\rangle)\\ &=\frac{1}{2}(\langle s_z+|\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}+\langle s_z-|\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}})\frac{1}{2}(\hat{S}_+(0)+\hat{S}_-(0))(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|s_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|s_z-\rangle)\\ &=\frac{1}{4}(\langle s_z+|\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}+\langle s_z-|\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}})(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\hbar|s_z-\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\hbar|s_z+\rangle)=\frac{\hbar}{4}(\mathrm{e}^{\mathrm{i}\omega t}+\mathrm{e}^{-\mathrm{i}\omega t})\\ &=\frac{\hbar}{4}(\cos\omega t+\mathrm{i}\sin\omega t+\cos\omega t-\mathrm{i}\sin\omega t)=\frac{\hbar}{2}\cos\omega t\end{aligned}$$

$$\begin{aligned}\langle\hat{S}_y\rangle(t)&=\langle u|\hat{S}_y(t)|u\rangle=[\frac{1}{\sqrt{2}}(\langle s_z+|+\langle s_z-|)]\mathrm{e}^{\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_y(0)\mathrm{e}^{-\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z(0)}[\frac{1}{\sqrt{2}}(|s_z+\rangle+|s_z-\rangle)]\\ &=\frac{1}{2}(\langle s_z+|\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}+\langle s_z-|\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}})\hat{S}_y(0)(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|s_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|s_z-\rangle)\\ &=\frac{1}{2}(\langle s_z+|\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}+\langle s_z-|\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}})\frac{1}{2\mathrm{i}}(\hat{S}_+(0)-\hat{S}_-(0))(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|s_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|s_z-\rangle)\\ &=\frac{1}{4\mathrm{i}}(\langle s_z+|\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}+\langle s_z-|\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}})(-\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\hbar|s_z-\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\hbar|s_z+\rangle)=\frac{\hbar}{4\mathrm{i}}(\mathrm{e}^{\mathrm{i}\omega t}-\mathrm{e}^{-\mathrm{i}\omega t})\\ &=\frac{\hbar}{4\mathrm{i}}(\cos\omega t+\mathrm{i}\sin\omega t-\cos\omega t+\mathrm{i}\sin\omega t)=\frac{\hbar}{2}\sin\omega t\end{aligned}$$

$$\begin{aligned}\langle\hat{S}_z\rangle(t)&=\langle u|\hat{S}_z(t)|u\rangle=[\frac{1}{\sqrt{2}}(\langle s_z+|+\langle s_z-|)]\hat{S}_z(0)[\frac{1}{\sqrt{2}}(|s_z+\rangle+|s_z-\rangle)]\\ &=\frac{1}{2}(\langle s_z+|+\langle s_z-|)(\frac{\hbar}{2}|s_z+\rangle-\frac{\hbar}{2}|s_z-\rangle)=0\end{aligned}$$

## 5.2 一个粒子的三维运动对应于哈密尔顿算符$\hat{H}=\frac{\hat{\boldsymbol{p}}^2}{2m}+V(\hat{\boldsymbol{x}})$，试通过计算$[\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}},\hat{H}]$获得$\frac{d \langle \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}} \rangle}{dt}=\langle \frac{\boldsymbol{p}^2}{m} \rangle-\langle \hat{\boldsymbol{x}} \cdot \nabla V \rangle$。如果方程左侧为零，得到维里定理的量子力学形式。在什么情况下是这样的结果？

**解**：用矢量的形式，我们可以得到$\hat{\boldsymbol{x}}=\hat{x}_i \boldsymbol{i}+\hat{x}_j \boldsymbol{j}+\hat{x}_k \boldsymbol{k}$，$\hat{\boldsymbol{p}}=\hat{p}_i \boldsymbol{i}+\hat{p}_j \boldsymbol{j}+\hat{p}_k \boldsymbol{k}$，因此$\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}}=\hat{x}_i \hat{p}_i+\hat{x}_j \hat{p}_j+\hat{x}_k \hat{p}_k$，$\hat{\boldsymbol{p}}^2=\hat{p}_i^2+\hat{p}_j^2+\hat{p}_k^2$，从而代入到$[\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}},\hat{H}]$，得：

$$\begin{aligned}[\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{p}},\hat{H}] &= [\hat{x}_i\hat{p}_i+\hat{x}_j\hat{p}_j+\hat{x}_k\hat{p}_k,\frac{\hat{\boldsymbol{p}}^2}{2m}+V(\hat{\boldsymbol{x}})] = [\hat{x}_i\hat{p}_i+\hat{x}_j\hat{p}_j+\hat{x}_k\hat{p}_k,\frac{\hat{p}_i^2+\hat{p}_j^2+\hat{p}_k^2}{2m}+V(\hat{\boldsymbol{x}})] \\ &= \frac{1}{2m}[\hat{x}_i\hat{p}_i+\hat{x}_j\hat{p}_j+\hat{x}_k\hat{p}_k,\hat{p}_i^2+\hat{p}_j^2+\hat{p}_k^2]+[\hat{x}_i\hat{p}_i+\hat{x}_j\hat{p}_j+\hat{x}_k\hat{p}_k,V(\hat{\boldsymbol{x}})]\end{aligned}$$

首先我们讨论第一项的结果，对于$u \in \{ i,j,k \}$，$v \in \{ i,j,k \}$，我们有

$$[\hat{x}_u\hat{p}_u,\hat{p}_v^2]=\hat{x}_u[\hat{p}_u,\hat{p}_v^2]+[\hat{x}_u,\hat{p}_v^2]\hat{p}_u=\hat{x}_u\cdot 0+([\hat{x}_u,\hat{p}_v]\hat{p}_v+\hat{p}_v[\hat{x}_u,\hat{p}_v])\hat{p}_u=2\mathrm{i}\hbar\delta_{uv}\hat{p}_v\hat{p}_u$$

因此第一项可以化简为

$$\frac{1}{2m}[\hat{x}_i\hat{p}_i+\hat{x}_j\hat{p}_j+\hat{x}_k\hat{p}_k,\hat{p}_i^2+\hat{p}_j^2+\hat{p}_k^2]=\frac{1}{2m}\sum_{\substack{u\in\{i,j,k\}\\ v\in\{i,j,k\}}}[\hat{x}_u\hat{p}_u,\hat{p}_v^2]=\frac{1}{2m}\sum_{\substack{u\in\{i,j,k\}\\ v\in\{i,j,k\}}}2\mathrm{i}\hbar\delta_{uv}\hat{p}_v\hat{p}_u=\frac{\mathrm{i}\hbar}{m}\sum_{u\in\{i,j,k\}}\hat{p}_u^2=\frac{\mathrm{i}\hbar}{m}\hat{\boldsymbol{p}}^2$$

接下来讨论第二项的结果，对于$u \in \{ i,j,k \}$，我们有

$$\begin{aligned}[\hat{x}_u\hat{p}_u,V(\hat{\boldsymbol{x}})] &= \hat{x}_u\hat{p}_uV(\hat{\boldsymbol{x}})-V(\hat{\boldsymbol{x}})\hat{x}_u\hat{p}_u=\hat{x}_u\hat{p}_uV(\boldsymbol{x})-V(\hat{\boldsymbol{x}})\hat{x}_u\hat{p}_u=\hat{x}_uV(\boldsymbol{x})\hat{p}_u+\hat{x}_u[-\mathrm{i}\hbar\nabla_{x_u}V(\boldsymbol{x})]-V(\hat{\boldsymbol{x}})\hat{x}_u\hat{p}_u \\ &= V(\hat{\boldsymbol{x}})\hat{x}_u\hat{x}_p-\mathrm{i}\hbar\hat{x}_u\nabla_{\hat{x}_u}V(\hat{\boldsymbol{x}})-V(\hat{\boldsymbol{x}})\hat{x}_u\hat{p}_u=-\mathrm{i}\hbar\hat{x}_u\nabla_{\hat{x}_u}V(\hat{\boldsymbol{x}})\end{aligned}$$

因此第二项可以化简为

$$[\hat{x}_i\hat{p}_i+\hat{x}_j\hat{p}_j+\hat{x}_k\hat{p}_k,V(\hat{\boldsymbol{x}})]=\sum_{u\in\{i,j,k\}}[\hat{x}_u\hat{p}_u,V(\hat{\boldsymbol{x}})]=-\mathrm{i}\hbar\sum_{u\in\{i,j,k\}}\hat{x}_u\nabla_{\hat{x}_u}V(\hat{\boldsymbol{x}})=-\mathrm{i}\hbar\hat{\boldsymbol{x}}\cdot\nabla V(\hat{\boldsymbol{x}})$$

最终我们可以得到$[\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}},\hat{H}]=\frac{\mathrm{i} \hbar}{m} \hat{\boldsymbol{p}}^2-\mathrm{i} \hbar \hat{\boldsymbol{x}} \cdot \nabla V(\hat{\boldsymbol{x}})$
回到本题，对$\langle \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}} \rangle$求导，得

$$\frac{d\langle\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{p}}\rangle}{dt}=\frac{1}{\mathrm{i}\hbar}\langle[\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{p}},\hat{H}]\rangle=\frac{1}{\mathrm{i}\hbar}\langle\frac{\mathrm{i}\hbar}{m}\hat{\boldsymbol{p}}^2-\mathrm{i}\hbar\hat{\boldsymbol{x}}\cdot\nabla V(\hat{\boldsymbol{x}})\rangle=\langle\frac{\hat{\boldsymbol{p}}^2}{m}\rangle-\langle\hat{\boldsymbol{x}}\cdot\nabla V\rangle$$

当$[\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}},\hat{H}]=0$时，即粒子处于定态时，方程左侧为零，从而得到维里定理的量子力学形式。

## 5.3 $t=0$时，一维自由粒子的波函数为一个高斯波包$\psi(x)=(\frac{1}{\sigma \sqrt{\pi}})^{\frac{1}{2}} \mathrm{e}^{-\frac{1}{2} (\frac{x}{\sigma})^2}$，在薛定谔表象中求解$t$时刻的波函数，与$\langle (\Delta x)^2 \rangle_t \langle (\Delta x)^2 \rangle_0 \geq \frac{\hbar^2 t^2}{4 m^2}$比较，说明波包随时间越来越弥散

**解**：对于一维自由粒子，其哈密尔顿算符为$\hat{H}=\frac{\hat{p}^2}{2m}$，因此时间演化算符可写作$\hat{U}=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \hat{H} t}=\mathrm{e}^{-\frac{\mathrm{i} t \hat{p}^2}{2m \hbar}}$，又根据傅里叶变换，得$\widetilde{\psi}(p,0)=(2 \pi \hbar)^{-\frac{1}{2}} \int^{+\infty}_{-\infty} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} p \cdot x} \psi(x,0) dx$（其中$\psi(x,0)$即$\psi(x)$），因此$\widetilde{\psi}(p,t)=\hat{U} \widetilde{\psi}(p,0)=\mathrm{e}^{-\frac{\mathrm{i} t p^2}{2m \hbar}} \widetilde{\psi}(p,0)$，再经傅里叶变换得$\psi(x,t)=(2 \pi \hbar)^{-\frac{1}{2}} \int^{+\infty}_{-\infty} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} p \cdot x} \widetilde{\psi}(p,t) dp$。现在我们来求解这些表达式：

$$
\begin{aligned}
\widetilde{\psi}(p,0) &= (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\cdot x}\psi(x,0)dx = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\cdot x}(\frac{1}{\sigma\sqrt{\pi}})^{\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}(\frac{x}{\sigma})^2}dx \\
&= (2\pi\hbar)^{-\frac{1}{2}}(\frac{1}{\sigma\sqrt{\pi}})^{\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{x^2}{2\sigma^2}-\frac{\mathrm{i}}{\hbar}px}dx = (2\pi\sqrt{\pi}\hbar\sigma)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{1}{2\sigma^2}(x+\frac{\mathrm{i}\sigma^2}{\hbar}p)^2-\frac{\sigma^2p^2}{2\hbar^2}}dx \\
&= (2\pi\sqrt{\pi}\hbar\sigma)^{-\frac{1}{2}}\mathrm{e}^{-\frac{\sigma^2p^2}{2\hbar^2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-(\frac{x+\frac{\mathrm{i}\sigma^2}{\hbar}p}{\sqrt{2}\sigma})^2}\cdot\sqrt{2}\sigma d(\frac{x+\frac{\mathrm{i}\sigma^2}{\hbar}p}{\sqrt{2}\sigma}) \\
&= (2\pi\sqrt{\pi}\hbar\sigma)^{-\frac{1}{2}}\mathrm{e}^{-\frac{\sigma^2p^2}{2\hbar^2}}\sqrt{2}\sigma\cdot\sqrt{\pi} = (\frac{\sigma}{\pi^{\frac{1}{2}}\hbar})^{\frac{1}{2}}\mathrm{e}^{-\frac{\sigma^2p^2}{2\hbar^2}}
\end{aligned}
$$

$$
\widetilde{\psi}(p,t) = \mathrm{e}^{-\frac{\mathrm{i}tp^2}{2m\hbar}}\widetilde{\psi}(p,0) = \mathrm{e}^{-\frac{\mathrm{i}tp^2}{2m\hbar}}\cdot(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar})^{\frac{1}{2}}\mathrm{e}^{-\frac{\sigma^2p^2}{2\hbar^2}} = (\frac{\sigma}{\pi^{\frac{1}{2}}\hbar})^{\frac{1}{2}}\mathrm{e}^{-(\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})p^2}
$$

$$
\begin{aligned}
\psi(x,t) &= (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p\cdot x}\widetilde{\psi}(p,t)dp = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p\cdot x}(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar})^{\frac{1}{2}}\mathrm{e}^{-(\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})p^2}dp \\
&= (2\pi\hbar)^{-\frac{1}{2}}(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar})^{\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-(\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})p^2+\frac{\mathrm{i}}{\hbar}p\cdot x}dp = (2\pi\hbar)^{-\frac{1}{2}}(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar})^{\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-(\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})(p-\frac{\frac{\mathrm{i}}{\hbar}x}{\frac{\mathrm{i}t}{m\hbar}+\frac{\sigma^2}{\hbar^2}})^2-\frac{x^2}{2\hbar^2(\frac{\mathrm{i}t}{m\hbar}+\frac{\sigma^2}{\hbar^2})}}dp \\
&= (\frac{\sigma}{2\pi^{\frac{3}{2}}\hbar^2})^{\frac{1}{2}}\mathrm{e}^{-\frac{x^2}{2\hbar^2(\frac{\mathrm{i}t}{m\hbar}+\frac{\sigma^2}{\hbar^2})}} \int_{-\infty}^{+\infty} \mathrm{e}^{-[\sqrt{\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}(p-\frac{\frac{\mathrm{i}}{\hbar}x}{\frac{\mathrm{i}t}{m\hbar}+\frac{\sigma^2}{\hbar^2}})]^2}\cdot\frac{1}{\sqrt{\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}}d[\sqrt{\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}(p-\frac{\frac{\mathrm{i}}{\hbar}x}{\frac{\mathrm{i}t}{m\hbar}+\frac{\sigma^2}{\hbar^2}})] \\
&= (\frac{\sigma}{2\pi^{\frac{3}{2}}\hbar^2})^{\frac{1}{2}}\mathrm{e}^{-\frac{x^2}{2\hbar^2(\frac{\mathrm{i}t}{m\hbar}+\frac{\sigma^2}{\hbar^2})}}\frac{1}{\sqrt{\frac{\mathrm{i}t}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}}\cdot\sqrt{\pi} = [\frac{1}{\sigma\pi^{\frac{1}{2}}(1+\frac{\mathrm{i}\hbar t}{m\sigma^2})}]^{\frac{1}{2}}\mathrm{e}^{-\frac{x^2}{2\sigma^2(1+\frac{\mathrm{i}\hbar t}{m\sigma^2})}}
\end{aligned}
$$

现在我们来求解$\langle (\Delta x)^2 \rangle_0$和$\langle (\Delta x)^2 \rangle_t$，显然

$$
\begin{aligned}
\langle x\rangle_0 &= \int_{-\infty}^{+\infty} x|\psi(x,0)|^2dx = \int_{-\infty}^{+\infty} \frac{x}{\sigma\sqrt{\pi}}\mathrm{e}^{-\frac{x^2}{\sigma^2}}dx = 0 \\
\langle x^2\rangle_0 &= \int_{-\infty}^{+\infty} x^2|\psi(x,0)|^2dx = \int_{-\infty}^{+\infty} \frac{x^2}{\sigma\sqrt{\pi}}\mathrm{e}^{-\frac{x^2}{\sigma^2}}dx = \frac{\sigma^2}{2}
\end{aligned}
$$

$$
\begin{aligned}
\langle x\rangle_t &= \int_{-\infty}^{+\infty} x|\psi(x,t)|^2dx = \int_{-\infty}^{+\infty} \frac{x}{\sigma\pi^{\frac{1}{2}}\sqrt{1-\frac{\hbar^2t^2}{m^2\sigma^4}}}\mathrm{e}^{-\frac{x^2}{\sigma^2(1-\frac{\hbar^2t^2}{m^2\sigma^4})}}dx = 0 \\
\langle x^2\rangle_t &= \int_{-\infty}^{+\infty} x^2|\psi(x,t)|^2dx = \int_{-\infty}^{+\infty} \frac{x^2}{\sigma\pi^{\frac{1}{2}}\sqrt{1+\frac{\hbar^2t^2}{m^2\sigma^4}}}\mathrm{e}^{-\frac{x^2}{\sigma^2(1+\frac{\hbar^2t^2}{m^2\sigma^4})}}dx = \frac{\sigma^2(1+\frac{\hbar^2t^2}{m^2\sigma^4})}{2}
\end{aligned}
$$

因此有

$$
\begin{aligned}
\langle(\Delta x)^2\rangle_0 &= \langle(x-\langle x\rangle_0)^2\rangle_0 = \langle x^2\rangle_0 - \langle x\rangle_0^2 = \frac{\sigma^2}{2} \\
\langle(\Delta x)^2\rangle_t &= \langle(x-\langle x\rangle_t)^2\rangle_t = \langle x^2\rangle_t - \langle x\rangle_t^2 = \frac{\sigma^2(1+\frac{\hbar^2t^2}{m^2\sigma^4})}{2} \\
\langle(\Delta x)^2\rangle_t\langle(\Delta x)^2\rangle_0 &= \frac{\sigma^2(1+\frac{\hbar^2t^2}{m^2\sigma^4})}{2}\frac{\sigma^2}{2} = \frac{\sigma^4}{4}+\frac{\hbar^2t^2}{4m^2} \geq \frac{\hbar^2t^2}{4m^2}
\end{aligned}
$$

**5.4 请用海森堡表象求解一维谐振子体系坐标与动量算符随时间演化的问题。如果初始状态是基态$\langle x | 0 \rangle$平移一段距离$s$，坐标与动量的平均值随时间的变化有什么特征？**

**解**：在海森堡表象下，算符微分为$\frac{d\hat{B}_H(t)}{dt}=\frac{1}{\mathrm{i} \hbar}[\hat{B}_H(t),\hat{H}]$，而一维谐振子体系的哈密尔顿算符为$\hat{H}=\frac{\hat{p}^2}{2m}+\frac{m \omega^2 \hat{x}^2}{2}$，因此有（记$\hat{x}_H(0) \equiv \hat{x}$，$\hat{p}_H(0) \equiv \hat{p}$）：

$$\frac{d\hat{x}_H(t)}{dt}=\frac{1}{\mathrm{i}\hbar}[\hat{x}_H(t),\hat{H}]=\frac{1}{\mathrm{i}\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}[\hat{x}_H(0),\frac{\hat{p}^2}{2m}+\frac{m\omega^2\hat{x}^2}{2}]\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=\frac{1}{\mathrm{i}\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\frac{\mathrm{i}\hbar\hat{p}}{m}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=\frac{\hat{p}_H(t)}{m}$$
$$\frac{d\hat{p}_H(t)}{dt}=\frac{1}{\mathrm{i}\hbar}[\hat{p}_H(t),\hat{H}]=\frac{1}{\mathrm{i}\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}[\hat{p}_H(0),\frac{\hat{p}^2}{2m}+\frac{m\omega^2\hat{x}^2}{2}]\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=\frac{1}{\mathrm{i}\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}(-\mathrm{i}\hbar m\omega^2\hat{x})\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}=-m\omega^2\hat{x}_H(t)$$

对两边分别求导，得$\begin{cases} \frac{d^2 \hat{x}_H(t)}{dt^2}=\frac{1}{m} \frac{d\hat{p}_H(t)}{dt}=-\omega^2 \hat{x}_H(t) \\ \frac{d^2 \hat{p}_H(t)}{dt^2}=-m \omega^2 \frac{d\hat{x}_H(t)}{dt}=-\omega^2 \hat{p}_H(t) \end{cases}$，相应的，这个方程组的通解为$\begin{cases} \hat{x}_H(t)=A \cos{\omega t}+B \sin{\omega t} \\ \hat{p}_H(t)=C \cos{\omega t}+D \sin{\omega t} \end{cases}$，对这个解求导得$\begin{cases} \frac{d\hat{x}_H(t)}{dt}=-\omega A \sin{\omega t}+\omega B \cos{\omega t} \\ \frac{d\hat{p}_H(t)}{dt}=-\omega C \sin{\omega t}+\omega D \cos{\omega t} \end{cases}$，当$t=0$时，根据上面的条件，可得：

$$\begin{cases} \hat{x}_H(0)=A \\ \hat{p}_H(0)=C \\ \frac{d\hat{x}_H(0)}{dt}=\omega B=\frac{\hat{p}_H(0)}{m} \\ \frac{d\hat{p}_H(0)}{dt}=\omega D=-m\omega^2\hat{x}_H(0) \end{cases} \Rightarrow \begin{cases} A=\hat{x} \\ B=\frac{\hat{p}}{m\omega} \\ C=\hat{p} \\ D=-m\omega\hat{x} \end{cases}$$

因此在海森堡表象下，坐标与动量算符为$\begin{cases} \hat{x}_H(t)=\hat{x} \cos{\omega t}+\frac{\hat{p}}{m \omega} \sin{\omega t} \\ \hat{p}_H(t)=\hat{p} \cos{\omega t}-m \omega \hat{x} \sin{\omega t} \end{cases}$，
当初始波函数为$\psi(x)=\langle x | 0^{'} \rangle=(\frac{1}{x_0 \sqrt{\pi}})^{\frac{1}{2}} \mathrm{e}^{-\frac{(x-s)^2}{2 x_0^2}}$（其中$x_0 \equiv \sqrt{\frac{\hbar}{m \omega}}$）时，对算符求平均值，得：

$$\begin{aligned}\langle\hat{x}\rangle(t)&=\langle 0^{'}|\hat{x}_H(t)|0^{'}\rangle=\int_{-\infty}^{+\infty}\langle 0^{'}|x\rangle\langle x|\hat{x}_H(t)|0^{'}\rangle dx=\int_{-\infty}^{+\infty}\langle 0^{'}|x\rangle\langle x|(\hat{x}\cos\omega t+\frac{\hat{p}}{m\omega}\sin\omega t)|0^{'}\rangle dx\\&=\cos\omega t\int_{-\infty}^{+\infty}x|\langle x|0^{'}\rangle|^2dx+\frac{\sin\omega t}{m\omega}\int_{-\infty}^{+\infty}\langle 0^{'}|x\rangle(-\mathrm{i}\hbar\nabla\langle x|0^{'}\rangle)dx\\&=\cos\omega t\int_{-\infty}^{+\infty}\frac{x}{x_0\sqrt{\pi}}\mathrm{e}^{-\frac{(x-s)^2}{x_0^2}}dx+\frac{\sin\omega t}{m\omega}\int_{-\infty}^{+\infty}(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}\mathrm{e}^{-\frac{(x-s)^2}{2x_0^2}}\cdot[-\mathrm{i}\hbar(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}\mathrm{e}^{-\frac{(x-s)^2}{2x_0^2}}\cdot(-\frac{x-s}{x_0^2})]dx\\&=s\cos wt\end{aligned}$$

$$\begin{aligned}\langle\hat{p}\rangle(t)&=\langle 0^{'}|\hat{p}_H(t)|0^{'}\rangle=\int_{-\infty}^{+\infty}\langle 0^{'}|x\rangle\langle x|\hat{p}_H(t)|0^{'}\rangle dx=\int_{-\infty}^{+\infty}\langle 0^{'}|x\rangle\langle x|(\hat{p}\cos\omega t-m\omega\hat{x}\sin\omega t)|0^{'}\rangle dx\\&=\cos\omega t\int_{-\infty}^{+\infty}\langle 0^{'}|x\rangle(-\mathrm{i}\hbar\nabla\langle x|0^{'}\rangle)dx-m\omega\sin\omega t\int_{-\infty}^{+\infty}x|\langle x|0^{'}\rangle|^2dx\\&=\cos\omega t\int_{-\infty}^{+\infty}(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}\mathrm{e}^{-\frac{(x-s)^2}{2x_0^2}}[-\mathrm{i}\hbar(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}\mathrm{e}^{-\frac{(x-s)^2}{2x_0^2}}\cdot(-\frac{x-s}{x_0^2})]dx-m\omega\sin\omega t\int_{-\infty}^{+\infty}\frac{x}{x_0\sqrt{\pi}}\mathrm{e}^{-\frac{(x-s)^2}{x_0^2}}dx\\&=-m\omega s\sin\omega t\end{aligned}$$

即坐标与动量的平均值随时间变化，分别呈余弦函数和正弦函数曲线

## 5.5 在海森堡表象中推导艾伦费斯特定理

**解**：在海森堡表象下，对算符$\hat{x}$在$t$时刻的期望值$\langle \hat{x} \rangle(t)$求关于时间$t$的导数，得（记海森堡表象下的态矢为$| u \rangle \equiv | u \rangle_H$）：

$$
\begin{aligned}
\frac{d}{dt}\langle\hat{x}\rangle(t) &= \frac{d}{dt}\langle u|\hat{x}_H(t)|u\rangle = \frac{d}{dt}\langle u|\hat{U}^\dagger(t)\hat{x}_H(0)\hat{U}(t)|u\rangle = \frac{d}{dt}\langle u|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{x}_H(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u\rangle \\
&= \langle u|\frac{\mathrm{i}}{\hbar}\hat{H}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{x}_H(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u\rangle + \langle u|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{x}_H(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}(-\frac{\mathrm{i}}{\hbar}\hat{H})|u\rangle \\
&= \frac{\mathrm{i}}{\hbar}\langle u|(\hat{H}\hat{x}_H(t)-\hat{x}_H(t)\hat{H})|u\rangle = \frac{1}{\mathrm{i}\hbar}\langle u|[\hat{x}_H(t),\hat{H}]|u\rangle
\end{aligned}
$$

而哈密尔顿算符可写作$\hat{H}=\frac{\hat{p}^2}{2m}+V(\hat{x})=\frac{\hat{p}_H(0)^2}{2m}+V(\hat{x}_H(0))$，因此代入得

$$
\begin{aligned}
\frac{d}{dt}\langle\hat{x}\rangle(t) &= \frac{\mathrm{i}}{\hbar}\langle u|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}[\hat{H}\hat{x}_H(0)-\hat{x}_H(0)\hat{H}]\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u\rangle \\
&= \frac{\mathrm{i}}{\hbar}\langle u|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\{[\frac{\hat{p}_H(0)^2}{2m}+V(\hat{x}_H(0))]\hat{x}_H(0)-\hat{x}_H(0)[\frac{\hat{p}_H(0)^2}{2m}+V(\hat{x}_H(0))]\}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u\rangle \\
&= \frac{\mathrm{i}}{\hbar}\langle u|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\{\frac{\hat{p}_H(0)^2}{2m}\hat{x}_H(0)-\hat{x}_H(0)\frac{\hat{p}_H(0)^2}{2m}\}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u\rangle \\
&= \frac{\mathrm{i}}{2\hbar m}\cdot(-2\mathrm{i}\hbar)\langle u|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{p}_H(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u\rangle = \frac{\langle\hat{p}_H(t)\rangle}{m} = \frac{\langle\hat{p}\rangle(t)}{m}
\end{aligned}
$$

## 5.6 证明$[\hat{x},F(\hat{p})]=\mathrm{i} \hbar \frac{\partial}{\partial \hat{p}} F(\hat{p})$，$[\hat{p},G(\hat{x})]=-\mathrm{i} \hbar \frac{\partial}{\partial \hat{x}} G(\hat{x})$

**证明**：首先我们证明$[\hat{x},\hat{p}^n]=\mathrm{i} \hbar n \hat{p}^{n-1}$，$[\hat{p},\hat{x}^n]=-\mathrm{i} \hbar n \hat{x}^{n-1}$，显然

$$
\begin{aligned}
[\hat{x},\hat{p}^n] &= \hat{x}\hat{p}^n-\hat{p}^n\hat{x} = ([\hat{x},\hat{p}]+\hat{p}\hat{x})\hat{p}^{n-1}-\hat{p}^n\hat{x} = (\mathrm{i}\hbar+\hat{p}\hat{x})\hat{p}^{n-1}-\hat{p}^n\hat{x} = \mathrm{i}\hbar\hat{p}^{n-1}+\hat{p}\hat{x}\hat{p}^{n-1}-\hat{p}^n\hat{x} \\
&= \mathrm{i}\hbar\hat{p}^{n-1}+\hat{p}([\hat{x},\hat{p}]+\hat{p}\hat{x})\hat{p}^{n-2}-\hat{p}^n\hat{x} = \mathrm{i}\hbar\hat{p}^{n-1}+\hat{p}(\mathrm{i}\hbar+\hat{p}\hat{x})\hat{p}^{n-2}-\hat{p}^n\hat{x} \\
&= 2\mathrm{i}\hbar\hat{p}^{n-1}+\hat{p}^2\hat{x}\hat{p}^{n-2}-\hat{p}^n\hat{x} = \cdots = \mathrm{i}\hbar n\hat{p}^{n-1}
\end{aligned}
$$

$$
\begin{aligned}
[\hat{p},\hat{x}^n] &= \hat{p}\hat{x}^n-\hat{x}^n\hat{p} = \hat{p}\hat{x}^n-\hat{x}^{n-1}([\hat{x},\hat{p}]+\hat{p}\hat{x}) = \hat{p}\hat{x}^n-\hat{x}^{n-1}(\mathrm{i}\hbar+\hat{p}\hat{x}) = \hat{p}\hat{x}^n-\mathrm{i}\hbar\hat{x}^{n-1}-\hat{x}^{n-1}\hat{p}\hat{x} \\
&= \hat{p}\hat{x}^n-\mathrm{i}\hbar\hat{x}^{n-1}-\hat{x}^{n-2}([\hat{x},\hat{p}]+\hat{p}\hat{x})\hat{x} = \hat{p}\hat{x}^n-\mathrm{i}\hbar\hat{x}^{n-1}-\hat{x}^{n-2}(\mathrm{i}\hbar+\hat{p}\hat{x})\hat{x} \\
&= \hat{p}\hat{x}^n-2\mathrm{i}\hbar\hat{x}^{n-1}-\hat{x}^{n-2}\hat{p}\hat{x}^2 = \cdots = -\mathrm{i}\hbar n\hat{x}^{n-1}
\end{aligned}
$$

接下来，将关于算符的函数展开，得$F(\hat{p})=\sum\limits_{i=0}^{\infty} c_i \hat{p}^i$，$G(\hat{x})=\sum\limits_{i=0}^{\infty} c_i \hat{x}^i$，因此

$$
[\hat{x},F(\hat{p})] = [\hat{x},\sum_{i=0}^{\infty}c_i\hat{p}^i] = \sum_{i=0}^{\infty}c_i[\hat{x},\hat{p}^i] = \sum_{i=0}^{\infty}c_i\mathrm{i}\hbar n\hat{p}^{n-1} = \mathrm{i}\hbar\sum_{i=0}^{\infty}c_i\frac{\partial\hat{p}^n}{\partial\hat{p}} = \mathrm{i}\hbar\frac{\partial\sum\limits_{i=0}^{\infty}c_i\hat{p}^n}{\partial\hat{p}} = \mathrm{i}\hbar\frac{\partial}{\partial\hat{p}}F(\hat{p})
$$

$$
[\hat{p},G(\hat{x})] = [\hat{p},\sum_{i=0}^{\infty}c_i\hat{x}^i] = \sum_{i=0}^{\infty}c_i[\hat{p},\hat{x}^i] = \sum_{i=0}^{\infty}c_i(-\mathrm{i}\hbar n\hat{x}^{n-1}) = -\mathrm{i}\hbar\sum_{i=0}^{\infty}c_i\frac{\partial\hat{x}^n}{\partial\hat{x}} = -\mathrm{i}\hbar\frac{\partial\sum\limits_{i=0}^{\infty}c_i\hat{x}^n}{\partial\hat{x}} = -\mathrm{i}\hbar\frac{\partial}{\partial\hat{x}}G(\hat{x})
$$

## 5.7 对于自旋1/2的体系，设其处在由0.7概率的$| s_x+ \rangle$态和0.3概率的$| s_y- \rangle$态所构成的混合态中，请根据$\hat{S}_z$的本征态表示出该混合态对应的密度算符及相应的密度矩阵

**解**：因为$| s_x+ \rangle=\frac{1}{\sqrt{2}}(| s_z+ \rangle+| s_z- \rangle)$，$| s_y- \rangle=\frac{1}{\sqrt{2}}(| s_z+ \rangle-\mathrm{i} | s_z- \rangle)$，所以题中混合态的密度算符为：

$$
\begin{aligned}
\hat{\rho} &= 0.7|s_x+\rangle\langle s_x+| + 0.3|s_y-\rangle\langle s_y-| \\
&= 0.7\cdot\frac{1}{\sqrt{2}}(|s_z+\rangle + |s_z-\rangle)\cdot\frac{1}{\sqrt{2}}(\langle s_z+| + \langle s_z-|) \\
&\quad + 0.3\cdot\frac{1}{\sqrt{2}}(|s_z+\rangle - \mathrm{i}|s_z-\rangle)\cdot\frac{1}{\sqrt{2}}(\langle s_z+| + \mathrm{i}\langle s_z-|) \\
&= 0.35(|s_z+\rangle\langle s_z+| + |s_z+\rangle\langle s_z-| + |s_z-\rangle\langle s_z+| + |s_z-\rangle\langle s_z-|) \\
&\quad + 0.15(|s_z+\rangle\langle s_z+| + \mathrm{i}|s_z+\rangle\langle s_z-| - \mathrm{i}|s_z-\rangle\langle s_z+| + |s_z-\rangle\langle s_z-|) \\
&= 0.5|s_z+\rangle\langle s_z+| + (0.35+0.15\mathrm{i})|s_z+\rangle\langle s_z-| + (0.35-0.15\mathrm{i})|s_z-\rangle\langle s_z+| + 0.5|s_z-\rangle\langle s_z-|
\end{aligned}
$$

写成密度矩阵的形式，即为$\boldsymbol{\rho}=\begin{pmatrix} 0.5&0.35+0.15 \mathrm{i} \\ 0.35-0.15 \mathrm{i}&0.5 \end{pmatrix}$