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

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

又知含时薛定谔方程为 $i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x}, t) = \hat{H}\psi(\boldsymbol{x}, t)$，取复共轭得 $-i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x}, t)^* = \hat{H}\psi(\boldsymbol{x}, t)^*$，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

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x}, t) = -\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x}, t) + V(\hat{\boldsymbol{x}})\psi(\boldsymbol{x}, t) \\ -i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x}, t)^* = -\frac{\hbar^2}{2m}\nabla_{\boldsymbol{x}}^2\psi(\boldsymbol{x}, t)^* + V(\hat{\boldsymbol{x}})\psi(\boldsymbol{x}, t)^* \end{cases}$$，从而

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

记概率通量为

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

则（此处用到边界条件）

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

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

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

解：由于 $\hat{O}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}_I(0)e^{-\frac{i}{\hbar}\hat{H}_0 t}$，因此对时间求导得

$$\frac{d\hat{O}_I(t)}{dt} = \frac{d[e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}_I(0)e^{-\frac{i}{\hbar}\hat{H}_0 t}]}{dt} = \frac{i}{\hbar}\big[\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}_I(0)e^{-\frac{i}{\hbar}\hat{H}_0 t} - e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}_I(0)e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0\big]$$
$$= \frac{i}{\hbar}\big[\hat{H}_0\hat{O}_I(t) - \hat{O}_I(t)\hat{H}_0\big] = \frac{1}{i\hbar}[\hat{O}_I(t), \hat{H}_0]$$

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 τ 足够大时的平均跃迁速率

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

$$c_n^{(2)}(\tau) = (-\frac{i}{\hbar})^2 \int_0^\tau dt_1 \int_0^{t_1} dt_2 \langle n|\hat{H}_I'(t_1)\hat{H}_I'(t_2)|i\rangle = (-\frac{i}{\hbar})^2 \sum_m \int_0^\tau dt_1 \int_0^{t_1} dt_2 \langle n|\hat{H}_I'(t_1)|m\rangle\langle m|\hat{H}_I'(t_2)|i\rangle$$

$$= -\frac{1}{\hbar^2}\sum_m \int_0^\tau dt_1 \int_0^{t_1} dt_2 e^{i\omega_{nm}t_1} V_{nm} e^{i\omega_{mi}t_2} V_{mi} = -\sum_m \frac{V_{nm}V_{mi}}{\hbar^2} \int_0^\tau e^{i\omega_{nm}t_1} dt_1 \int_0^{t_1} e^{i\omega_{mi}t_2} dt_2$$

$$= -\sum_m \frac{V_{nm}V_{mi}}{\hbar^2} \int_0^\tau e^{i\omega_{nm}t_1} dt_1 \cdot (\frac{e^{i\omega_{mi}t_1}-1}{i\omega_{mi}}) = -\sum_m \frac{V_{nm}V_{mi}}{i\hbar^2\omega_{mi}} \int_0^\tau [e^{i(\omega_{nm}+\omega_{mi})t_1} - e^{i\omega_{nm}t_1}]dt_1$$

$$= -\sum_m \frac{V_{nm}V_{mi}}{i\hbar^2\omega_{mi}}[\frac{e^{i(\omega_{nm}+\omega_{mi})\tau}-1}{i(\omega_{nm}+\omega_{mi})} - \frac{e^{i\omega_{nm}\tau}-1}{i\omega_{nm}}] = -\sum_m \frac{V_{nm}V_{mi}}{i\hbar^2\omega_{mi}}[\frac{e^{i\omega_{ni}\tau}-1}{i\omega_{ni}} - \frac{e^{i\omega_{nm}\tau}-1}{i\omega_{nm}}]$$

$$= -\sum_m \frac{V_{nm}V_{mi}}{i\hbar^2\omega_{mi}}[e^{\frac{i\omega_{ni}\tau}{2}}\frac{e^{\frac{i\omega_{ni}\tau}{2}}-e^{-\frac{i\omega_{ni}\tau}{2}}}{i\omega_{ni}} - e^{\frac{i\omega_{nm}\tau}{2}}\frac{e^{\frac{i\omega_{nm}\tau}{2}}-e^{-\frac{i\omega_{nm}\tau}{2}}}{i\omega_{nm}}]$$

$$= \sum_m \frac{iV_{nm}V_{mi}}{\hbar^2\omega_{mi}}[e^{\frac{i\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}} - e^{\frac{i\omega_{nm}\tau}{2}}\frac{\sin\frac{\omega_{nm}\tau}{2}}{\frac{\omega_{nm}}{2}}]$$

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

$$P_{i\to n}^{(2)}(\tau) = |c_n^{(1)}(\tau) + c_n^{(2)}(\tau)|^2 = \Big| -\frac{iV_{ni}}{\hbar}e^{\frac{i\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}} + \sum_m \frac{iV_{nm}V_{mi}}{\hbar^2\omega_{mi}}[e^{\frac{i\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}} - e^{\frac{i\omega_{nm}\tau}{2}}\frac{\sin\frac{\omega_{nm}\tau}{2}}{\frac{\omega_{nm}}{2}}]\Big|^2$$

$$= \Big|(-\frac{iV_{ni}}{\hbar} + \sum_m \frac{iV_{nm}V_{mi}}{\hbar^2\omega_{mi}})e^{\frac{i\omega_{ni}\tau}{2}}\frac{\sin\frac{\omega_{ni}\tau}{2}}{\frac{\omega_{ni}}{2}} - \sum_m \frac{iV_{nm}V_{mi}}{\hbar^2\omega_{mi}}e^{\frac{i\omega_{nm}\tau}{2}}\frac{\sin\frac{\omega_{nm}\tau}{2}}{\frac{\omega_{nm}}{2}}\Big|^2$$

$$= \Big| -\frac{V_{ni}}{\hbar} + \sum_m \frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2 \frac{\sin^2\frac{\omega_{ni}\tau}{2}}{(\frac{\omega_{ni}}{2})^2} + \sum_m \Big|\frac{V_{nm}V_{mi}}{\hbar^2\omega_{mi}}\Big|^2 \frac{\sin^2\frac{\omega_{nm}\tau}{2}}{(\frac{\omega_{nm}}{2})^2} + 交叉项$$

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

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

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

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

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

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

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：

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

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

$$\hat{S}_z(t) = \hat{U}^\dagger(t)\hat{S}_z(0)\hat{U}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{S}_z(0)e^{-\frac{i}{\hbar}\hat{H}t} = e^{\frac{i\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_z(0)e^{-\frac{i\omega t}{\hbar}\hat{S}_z(0)} = \hat{S}_z(0)$$

因此t时刻各个自旋算符的期望值为

$$\langle\hat{S}_x\rangle(t) = \langle u|\hat{S}_x(t)|u\rangle = [\frac{1}{\sqrt{2}}(\langle s_z + | + \langle s_z - |)]e^{\frac{i\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_x(0)e^{-\frac{i\omega t}{\hbar}\hat{S}_z(0)}[\frac{1}{\sqrt{2}}(|s_z+\rangle + |s_z-\rangle)]$$

$$= \frac{1}{2}(\langle s_z + |e^{\frac{i\omega t}{2}} + \langle s_z - |e^{-\frac{i\omega t}{2}})\hat{S}_x(0)(e^{-\frac{i\omega t}{2}}|s_z+\rangle + e^{\frac{i\omega t}{2}}|s_z-\rangle)$$

$$= \frac{1}{2}(\langle s_z + |e^{\frac{i\omega t}{2}} + \langle s_z - |e^{-\frac{i\omega t}{2}})\frac{1}{2}(\hat{S}_+(0) + \hat{S}_-(0))(e^{-\frac{i\omega t}{2}}|s_z+\rangle + e^{\frac{i\omega t}{2}}|s_z-\rangle)$$

$$= \frac{1}{4}(\langle s_z + |e^{\frac{i\omega t}{2}} + \langle s_z - |e^{-\frac{i\omega t}{2}})(e^{-\frac{i\omega t}{2}}\hbar|s_z-\rangle + e^{\frac{i\omega t}{2}}\hbar|s_z+\rangle) = \frac{\hbar}{4}(e^{i\omega t} + e^{-i\omega t})$$

$$= \frac{\hbar}{4}(\cos\omega t + i\sin\omega t + \cos\omega t - i\sin\omega t) = \frac{\hbar}{2}\cos\omega t$$

$$\langle\hat{S}_y\rangle(t) = \langle u|\hat{S}_y(t)|u\rangle = [\frac{1}{\sqrt{2}}(\langle s_z + | + \langle s_z - |)]e^{\frac{i\omega t}{\hbar}\hat{S}_z(0)}\hat{S}_y(0)e^{-\frac{i\omega t}{\hbar}\hat{S}_z(0)}[\frac{1}{\sqrt{2}}(|s_z+\rangle + |s_z-\rangle)]$$

$$= \frac{1}{2}(\langle s_z + |e^{\frac{i\omega t}{2}} + \langle s_z - |e^{-\frac{i\omega t}{2}})\hat{S}_y(0)(e^{-\frac{i\omega t}{2}}|s_z+\rangle + e^{\frac{i\omega t}{2}}|s_z-\rangle)$$

$$= \frac{1}{2}(\langle s_z + |e^{\frac{i\omega t}{2}} + \langle s_z - |e^{-\frac{i\omega t}{2}})\frac{1}{2i}(\hat{S}_+(0) - \hat{S}_-(0))(e^{-\frac{i\omega t}{2}}|s_z+\rangle + e^{\frac{i\omega t}{2}}|s_z-\rangle)$$

$$= \frac{1}{4i}(\langle s_z + |e^{\frac{i\omega t}{2}} + \langle s_z - |e^{-\frac{i\omega t}{2}})(-e^{-\frac{i\omega t}{2}}\hbar|s_z-\rangle + e^{\frac{i\omega t}{2}}\hbar|s_z+\rangle) = \frac{\hbar}{4i}(e^{i\omega t} - e^{-i\omega t})$$

$$= \frac{\hbar}{4i}(\cos\omega t + i\sin\omega t - \cos\omega t + i\sin\omega t) = \frac{\hbar}{2}\sin\omega t$$

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

$$= \frac{1}{2}(\langle s_z + | + \langle s_z - |)(\frac{\hbar}{2}|s_z+\rangle - \frac{\hbar}{2}|s_z-\rangle) = 0$$

5.2 一个粒子的三维运动对应于哈密尔顿算符$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$，试通过计算$[\hat{x}\cdot\hat{p}, \hat{H}]$获得$\frac{d\langle\hat{x}\cdot\hat{p}\rangle}{dt} = \langle\frac{p^2}{m}\rangle - \langle\hat{x}\cdot\nabla V\rangle$。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$\hat{x} = \hat{x}_i\boldsymbol{i} + \hat{x}_j\boldsymbol{j} + \hat{x}_k\boldsymbol{k}$，$\hat{p} = \hat{p}_i\boldsymbol{i} + \hat{p}_j\boldsymbol{j} + \hat{p}_k\boldsymbol{k}$，因此$\hat{x}\cdot\hat{p} = \hat{x}_i\hat{p}_i + \hat{x}_j\hat{p}_j + \hat{x}_k\hat{p}_k$，$\hat{p}^2 = \hat{p}_i^2 + \hat{p}_j^2 + \hat{p}_k^2$，从而代入到$[\hat{x}\cdot\hat{p}, \hat{H}]$，得：

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

$$= \frac{1}{2m}[\hat{x}_i\hat{p}_i + \hat{x}_j\hat{p}_j + \hat{x}_k\hat{p}_k, \hat{p}_i^2 + \hat{p}_j^2 + \hat{p}_k^2] + [\hat{x}_i\hat{p}_i + \hat{x}_j\hat{p}_j + \hat{x}_k\hat{p}_k, V(\hat{x})]$$

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

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

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

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

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$\langle(\Delta x)^2\rangle_t\langle(\Delta x)^2\rangle_0 \geq \frac{\hbar^2 t^2}{4m^2}$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$\widetilde{\psi}(p,t) = \hat{U}\widetilde{\psi}(p,0) = \mathrm{e}^{-\frac{\mathrm{i}tp^2}{2m\hbar}}\widetilde{\psi}(p,0)$，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：

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

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

$$\psi(x,t) = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{\frac{i}{\hbar}p\cdot x}\widetilde{\psi}(p,t)dp = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{\frac{i}{\hbar}p\cdot x}\big(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar}\big)^{\frac{1}{2}} \mathrm{e}^{-(\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})p^2}dp$$

$$= (2\pi\hbar)^{-\frac{1}{2}}\big(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar}\big)^{\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-(\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})p^2+\frac{i}{\hbar}p\cdot x}dp = (2\pi\hbar)^{-\frac{1}{2}}\big(\frac{\sigma}{\pi^{\frac{1}{2}}\hbar}\big)^{\frac{1}{2}} \int_{-\infty}^{+\infty} \mathrm{e}^{-(\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2})(p-\frac{\frac{i}{\hbar}x}{\frac{it}{m\hbar}+\frac{\sigma^2}{\hbar^2}})^2-\frac{x^2}{2\hbar^2(\frac{it}{m\hbar}+\frac{\sigma^2}{\hbar^2})}}dp$$

$$= \big(\frac{\sigma}{2\pi^{\frac{3}{2}}\hbar^2}\big)^{\frac{1}{2}} \mathrm{e}^{-\frac{x^2}{2\hbar^2(\frac{it}{m\hbar}+\frac{\sigma^2}{\hbar^2})}} \int_{-\infty}^{+\infty} \mathrm{e}^{-[\sqrt{\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}(p-\frac{\frac{i}{\hbar}x}{\frac{it}{m\hbar}+\frac{\sigma^2}{\hbar^2}})]^2} \cdot \frac{1}{\sqrt{\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}}d[\sqrt{\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}(p-\frac{\frac{i}{\hbar}x}{\frac{it}{m\hbar}+\frac{\sigma^2}{\hbar^2}})]$$

$$= \big(\frac{\sigma}{2\pi^{\frac{3}{2}}\hbar^2}\big)^{\frac{1}{2}} \mathrm{e}^{-\frac{x^2}{2\hbar^2(\frac{it}{m\hbar}+\frac{\sigma^2}{\hbar^2})}} \frac{1}{\sqrt{\frac{it}{2m\hbar}+\frac{\sigma^2}{2\hbar^2}}} \cdot \sqrt{\pi} = [\frac{1}{\sigma\pi^{\frac{1}{2}}(1+\frac{i\hbar t}{m\sigma^2})}]^{\frac{1}{2}} \mathrm{e}^{-\frac{x^2}{2\sigma^2(1+\frac{i\hbar t}{m\sigma^2})}}$$

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

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

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

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

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

因此有

$$\langle(\Delta x)^2\rangle_0 = \langle(x-\langle x\rangle_0)^2\rangle_0 = \langle x^2\rangle_0 - \langle x\rangle_0^2 = \frac{\sigma^2}{2}$$

$$\langle(\Delta x)^2\rangle_t = \langle(x-\langle x\rangle_t)^2\rangle_t = \langle x^2\rangle_t - \langle x\rangle_t^2 = \frac{\sigma^2(1+\frac{\hbar^2 t^2}{m^2\sigma^4})}{2}$$

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

5.4 请用海森堡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$\frac{d\hat{B}_H(t)}{dt} = \frac{1}{i\hbar}[\hat{B}_H(t),\hat{H}]$，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$\hat{x}_H(0) \equiv \hat{x}$, $\hat{p}_H(0) \equiv \hat{p}$）：

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

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

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 $\psi(x) = \langle x|0'\rangle = (\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}} e^{-\frac{(x-s)^2}{2x_0^2}}$ （其中 $x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$）时，对算符求平均值，得：

$$\langle\hat{x}\rangle(t) = \langle 0'|\hat{x}_H(t)|0'\rangle = \int_{-\infty}^{+\infty}\langle 0'|x\rangle\langle x|\hat{x}_H(t)|0'\rangle dx = \int_{-\infty}^{+\infty}\langle 0'|x\rangle\langle x|(\hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t)|0'\rangle dx$$

$$= \cos\omega t \int_{-\infty}^{+\infty} x|\langle x|0'\rangle|^2 dx + \frac{\sin\omega t}{m\omega}\int_{-\infty}^{+\infty}\langle 0'|x\rangle(-i\hbar\nabla\langle x|0'\rangle)dx$$

$$= \cos\omega t \int_{-\infty}^{+\infty} \frac{x}{x_0\sqrt{\pi}}e^{-\frac{(x-s)^2}{x_0^2}}dx + \frac{\sin\omega t}{m\omega}\int_{-\infty}^{+\infty}(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}e^{-\frac{(x-s)^2}{2x_0^2}}\cdot[-i\hbar(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}e^{-\frac{(x-s)^2}{2x_0^2}}\cdot(-\frac{x-s}{x_0^2})]dx$$

$$= s\cos wt$$

$$\langle\hat{p}\rangle(t) = \langle 0'|\hat{p}_H(t)|0'\rangle = \int_{-\infty}^{+\infty}\langle 0'|x\rangle\langle x|\hat{p}_H(t)|0'\rangle dx = \int_{-\infty}^{+\infty}\langle 0'|x\rangle\langle x|(\hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t)|0'\rangle dx$$

$$= \cos\omega t \int_{-\infty}^{+\infty}\langle 0'|x\rangle(-i\hbar\nabla\langle x|0'\rangle)dx - m\omega\sin\omega t \int_{-\infty}^{+\infty} x|\langle x|0'\rangle|^2 dx$$

$$= \cos\omega t \int_{-\infty}^{+\infty}(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}e^{-\frac{(x-s)^2}{2x_0^2}}[-i\hbar(\frac{1}{x_0\sqrt{\pi}})^{\frac{1}{2}}e^{-\frac{(x-s)^2}{2x_0^2}}\cdot(-\frac{x-s}{x_0^2})]dx - m\omega\sin\omega t\int_{-\infty}^{+\infty}\frac{x}{x_0\sqrt{\pi}}e^{-\frac{(x-s)^2}{x_0^2}}dx$$

$$= -m\omega s\sin\omega t$$

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 $|u\rangle \equiv |u\rangle_H$）：

$$\frac{d}{dt}\langle\hat{x}\rangle(t) = \frac{d}{dt}\langle u|\hat{x}_H(t)|u\rangle = \frac{d}{dt}\langle u|\hat{U}^\dagger(t)\hat{x}_H(0)\hat{U}(t)|u\rangle = \frac{d}{dt}\langle u|e^{\frac{i}{\hbar}\hat{H}t}\hat{x}_H(0)e^{-\frac{i}{\hbar}\hat{H}t}|u\rangle$$

$$= \langle u|\frac{i}{\hbar}\hat{H}e^{\frac{i}{\hbar}\hat{H}t}\hat{x}_H(0)e^{-\frac{i}{\hbar}\hat{H}t}|u\rangle + \langle u|e^{\frac{i}{\hbar}\hat{H}t}\hat{x}_H(0)e^{-\frac{i}{\hbar}\hat{H}t}(-\frac{i}{\hbar}\hat{H})|u\rangle$$

$$= \frac{i}{\hbar}\langle u|(\hat{H}\hat{x}_H(t) - \hat{x}_H(t)\hat{H})|u\rangle = \frac{1}{i\hbar}\langle u|[\hat{x}_H(t),\hat{H}]|u\rangle$$

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

$$\frac{d}{dt}\langle\hat{x}\rangle(t) = \frac{i}{\hbar}\langle u|e^{\frac{i}{\hbar}\hat{H}t}[\hat{H}\hat{x}_H(0) - \hat{x}_H(0)\hat{H}]e^{-\frac{i}{\hbar}\hat{H}t}|u\rangle$$

$$= \frac{i}{\hbar}\langle u|e^{\frac{i}{\hbar}\hat{H}t}\{[\frac{\hat{p}_H(0)^2}{2m} + V(\hat{x}_H(0))]\hat{x}_H(0) - \hat{x}_H(0)[\frac{\hat{p}_H(0)^2}{2m} + V(\hat{x}_H(0))]\}e^{-\frac{i}{\hbar}\hat{H}t}|u\rangle$$

$$= \frac{i}{\hbar}\langle u|e^{\frac{i}{\hbar}\hat{H}t}\{\frac{\hat{p}_H(0)^2}{2m}\hat{x}_H(0) - \hat{x}_H(0)\frac{\hat{p}_H(0)^2}{2m}\}e^{-\frac{i}{\hbar}\hat{H}t}|u\rangle$$

$$= \frac{i}{2\hbar m}\cdot(-2i\hbar)\langle u|e^{\frac{i}{\hbar}\hat{H}t}\hat{p}_H(0)e^{-\frac{i}{\hbar}\hat{H}t}|u\rangle = \frac{\langle\hat{p}_H(t)\rangle}{m} = \frac{\langle\hat{p}\rangle(t)}{m}$$

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

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

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

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

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

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

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

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：

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

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