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

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

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：

5.2 一个粒子的三维运动对应于哈密尔顿算符$\hat{H}=\frac{\boldsymbol{p}^2}{2m}+V(\hat{\boldsymbol{x}})$，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：

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$\langle(\Delta x)^2\rangle_t\langle(\Delta x)^2\rangle_0\geq\frac{\hbar^2t^2}{4m^2}$比较，说明波包随时间越来越弥散

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?

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$\boldsymbol{\rho}=\begin{pmatrix}0.5&0.35+0.15\mathrm{i}\\0.35-0.15\mathrm{i}&0.5\end{pmatrix}$