

第 1 题 (课本习题 1.29) 得分: _____. (a) Gottfried (1966) 在他的书的 247 页上说: 对所有能表示成其宗量的幂级数的函数 F 和 G , 从基本对易关系都可以“容易地推导”出

$$[x_i, G(\mathbf{p})] = i\hbar \frac{\partial G}{\partial p_i}, \quad [p_i, F(\mathbf{x})] = -i\hbar \frac{\partial F}{\partial x_i}$$

证明这个说法.

(b) 求 $[x^2, p^2]$ 的值, 把你的结果与经典的泊松括号 $[x^2, p^2]_{\text{经典}}$ 相比较.

解: (a) 通过泰勒展开将函数 F 和 G 分别表为其宗量的幂级数和

$$F(\mathbf{x}) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \binom{n+m+l}{n} \binom{m+l}{m} \frac{1}{(n+m+l)!} \frac{\partial^{n+m+l} F}{\partial x_i^n \partial x_j^m \partial x_k^l} x_i^n x_j^m x_k^l \equiv \sum_{nml} f_{nml} x_i^n x_j^m x_k^l, \quad (1)$$

$$G(\mathbf{p}) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \binom{n+m+l}{n} \binom{m+l}{m} \frac{1}{(n+m+l)!} \frac{\partial^{n+m+l} G}{\partial p_i^n \partial p_j^m \partial p_k^l} p_i^n p_j^m p_k^l \equiv \sum_{nml} g_{nml} p_i^n p_j^m p_k^l \quad (2)$$

利用基本对易关系

$$[x_i, p_j] = i\hbar \delta_{ij}, \quad (3)$$

有

$$\begin{aligned} [x_i, p_i^n] &= p_i [x_i, p_i^{n-1}] + [x_i, p_i] p_i^{n-1} = p_i [x_i, p_i^{n-1}] + i\hbar p_i^{n-1} \\ &= p_i^2 [x_i, p_i^{n-2}] + p_i [x_i, p_i] p_i^{n-2} + i\hbar p_i^{n-1} = p_i^2 [x_i, p_i^{n-2}] + 2i\hbar p_i^{n-1} \\ &\dots \\ &= ni\hbar p_i^{n-1}, \end{aligned} \quad (4)$$

$$\begin{aligned} [p_i, x_i^n] &= x_i [p_i, x_i^{n-1}] + [p_i, x_i] x_i^{n-1} = x_i [p_i, x_i^{n-1}] - i\hbar x_i^{n-1} \\ &= x_i^2 [p_i, x_i^{n-2}] + x_i [p_i, x_i] x_i^{n-2} - i\hbar x_i^{n-1} = x_i^2 [p_i, x_i^{n-2}] - 2i\hbar x_i^{n-1} \\ &\dots \\ &= -ni\hbar x_i^{n-1}, \end{aligned} \quad (5)$$

从而

$$[x_i, G(\mathbf{p})] = [x_i, \sum_{nml} g_{nml} p_i^n p_j^m p_k^l] = \sum_{nml} g_{nml} [x_i, p_i^n] p_j^m p_k^l = i\hbar \sum_{nml} g_{nml} n p_i^{n-1} p_j^m p_k^l = i\hbar \frac{\partial G}{\partial p_i}, \quad (6)$$

$$[p_i, F(\mathbf{x})] = [p_i, \sum_{nml} f_{nml} x_i^n x_j^m x_k^l] = \sum_{nml} f_{nml} [p_i, x_i^n] x_j^m x_k^l = -i\hbar \sum_{nml} f_{nml} n x_i^{n-1} x_j^m x_k^l = -i\hbar \frac{\partial F}{\partial x_i}. \quad (7)$$

(b)

$$[x^2, p^2] = x[x, p^2] + [x, p^2]x = x\{p[x, p] + [x, p], p\} + \{p[x, p] + [x, p], p\}x = 2i\hbar(xp + px) \quad (8)$$

经典的泊松括号:

$$[x^2, p^2]_{\text{经典}} = \frac{\partial x^2}{\partial x} \frac{\partial p^2}{\partial p} - \frac{\partial x^2}{\partial p} \frac{\partial p^2}{\partial x} = 4xp. \quad (9)$$

只需将经典的泊松括号厄米化, 即可得到与量子力学中一致的形式:

$$[x^2, p^2]_{\text{经典}} = 4xp \xrightarrow{\text{厄米化}} 2xp + 2px = \frac{1}{i\hbar} [x^2, p^2]. \quad (10)$$

□

第 2 题 (课本习题 1.31) 得分: _____. 在正文中我们讨论了 $\mathcal{T}(\mathbf{d}\mathbf{x}')$ 在位置和动量本征右矢上以及在一个更一般的态右矢 $|\alpha\rangle$ 的效应. 我们还可以研究期待值 $\langle \mathbf{x} \rangle$ 和 $\langle \mathbf{p} \rangle$ 在无穷小平移下的行为. 利用 (1.6.25) 式和 (1.6.45) 式并令 $|\alpha\rangle \rightarrow \mathcal{T}(\mathbf{d}\mathbf{x}')|\alpha\rangle$, 证明在无穷小平移下 $\langle \mathbf{x} \rangle \rightarrow \langle \mathbf{x} \rangle + \mathbf{d}\mathbf{x}'$, $\langle \mathbf{p} \rangle \rightarrow \langle \mathbf{p} \rangle$.

证: 平移前,

$$\langle \mathbf{x} \rangle = \langle \alpha | \mathbf{x} | \alpha \rangle, \quad (11)$$

$$\langle \mathbf{p} \rangle = \langle \alpha | \mathbf{p} | \alpha \rangle. \quad (12)$$

平移后, 利用 (1.6.25) 式 $[\mathbf{x}, \mathcal{T}(\mathbf{d}\mathbf{x}')] = \mathbf{d}\mathbf{x}'$, 有

$$\begin{aligned} \langle \alpha | \mathcal{T}^\dagger(\mathbf{d}\mathbf{x}') \mathbf{x} \mathcal{T}(\mathbf{d}\mathbf{x}') | \alpha \rangle &= \langle \alpha | \mathcal{T}^\dagger(\mathbf{d}\mathbf{x}') [\mathcal{T}(\mathbf{d}\mathbf{x}') \mathbf{x} + \mathbf{d}\mathbf{x}'] | \alpha \rangle \\ &= \langle \alpha | \mathcal{T}^\dagger(\mathbf{d}\mathbf{x}') \mathcal{T}(\mathbf{d}\mathbf{x}') \mathbf{x} | \alpha \rangle + \langle \alpha | \mathcal{T}^\dagger(\mathbf{d}\mathbf{x}') \mathbf{d}\mathbf{x}' | \alpha \rangle \\ &= \langle \alpha | \mathbf{x} | \alpha \rangle + \langle \alpha | (1 + i\mathbf{K} \cdot \mathbf{d}\mathbf{x}') \mathbf{d}\mathbf{x}' | \alpha \rangle \\ &\quad (\text{略去高阶小量}) \\ &= \langle \mathbf{x} \rangle + \langle \alpha | \mathbf{d}\mathbf{x}' | \alpha \rangle \\ &= \langle \mathbf{x} \rangle + \mathbf{d}\mathbf{x}', \end{aligned} \quad (13)$$

由于平移算符 $\mathcal{T}(\mathbf{d}\mathbf{x}')$ 可表为动量算符 \mathbf{p} 的幂级数之和, 利用 (1.6.45) 式 $[p_i, p_j] = 0$, 有 $[\mathcal{T}(\mathbf{d}\mathbf{x}'), \mathbf{p}] = 0$, 从而

$$\langle \alpha | \mathcal{T}^\dagger(\mathbf{d}\mathbf{x}') \mathbf{p} \mathcal{T}(\mathbf{d}\mathbf{x}') | \alpha \rangle = \langle \alpha | \mathcal{T}^\dagger(\mathbf{d}\mathbf{x}') \mathcal{T}(\mathbf{d}\mathbf{x}') \mathbf{p} | \alpha \rangle = \langle \alpha | \mathbf{p} | \alpha \rangle = \langle \mathbf{p} \rangle. \quad (14)$$

□

第 3 题 (课本习题 1.33) 得分: _____. (a) 证明下列各式:

i. $\langle p' | x | \alpha \rangle = i\hbar \frac{\partial}{\partial p'} \langle p' | \alpha \rangle.$

ii. $\langle \beta | x | \alpha \rangle = \int dp' \phi_\beta^*(p') i\hbar \frac{\partial}{\partial p'} \phi_\alpha(p'),$ 其中 $\phi_\alpha(p') = \langle p' | \alpha \rangle$ 和 $\phi_\beta(p') = \langle p' | \beta \rangle$ 都是动量空间波函数.

(b)

$$\exp\left(\frac{ix\Xi}{\hbar}\right)$$

的物理意义是什么, 其中 x 是位置算符, 而 Ξ 是某个量纲为动量的数? 证明你的答案的正确性.

证: (a) i.

$$\langle p' | x | \alpha \rangle = \int dp'' \langle p' | x | p'' \rangle \langle p'' | \alpha \rangle, \quad (15)$$

其中

$$\begin{aligned} \langle p' | x | p'' \rangle &= \int dx' \langle p' | x | x' \rangle \langle x' | p'' \rangle \\ &= \int dx' x' \langle p' | x' \rangle \langle x' | p'' \rangle \\ &= \frac{1}{2\pi\hbar} \int dx' x' \exp\left[-i\frac{(p' - p'')x'}{\hbar}\right] \\ &= \frac{1}{2\pi\hbar} \int dx' i\hbar \frac{\partial}{\partial p'} \exp\left[-i\frac{(p' - p'')x'}{\hbar}\right] \\ &= i\hbar \frac{\partial}{\partial p'} \frac{1}{2\pi\hbar} \int dx' \exp\left[-i\frac{(p' - p'')x'}{\hbar}\right] \end{aligned}$$

$$=i\hbar\frac{\partial}{\partial p'}\delta(p'-p''), \quad (16)$$

故

$$\langle p'|x|\alpha\rangle = \int dp'' i\hbar\frac{\partial}{\partial p'}\delta(p'-p'')\langle p''|\alpha\rangle = i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle. \quad (17)$$

ii.

$$\langle\beta|x|\alpha\rangle = \int dp' \langle\beta|p'\rangle\langle p'|x|\alpha\rangle = \int dp' \langle\beta|p'\rangle i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle = \int dp' \phi_\beta^*(p')i\hbar\frac{\partial}{\partial p'}\phi_\alpha(p'). \quad (18)$$

(b) $\exp\left(\frac{ix\Xi}{\hbar}\right)$ 为动量平移算符. 证明如下:

将 $\exp\left(\frac{ix\Xi}{\hbar}\right)$ 作用于动量算符 p 的本征态 $|p'\rangle$ 后, 其动量变为 $p' + \Xi$:

$$\begin{aligned} p \exp\left(\frac{ix\Xi}{\hbar}\right) |p'\rangle &= p \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{ix\Xi}{\hbar}\right)^n |p'\rangle \\ &\quad (\text{利用第 1 题中推得的对易关系: } [p, x^n] = -ni\hbar x^{n-1}) \\ &= \left[\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{ix\Xi}{\hbar}\right)^n p + \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(\frac{ix\Xi}{\hbar}\right)^{n-1} \Xi \right] |p'\rangle \\ &= (p' + \Xi) \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{ix\Xi}{\hbar}\right)^n |p'\rangle \\ &= (p' + \Xi) \exp\left(\frac{ix\Xi}{\hbar}\right) |p'\rangle, \end{aligned} \quad (19)$$

故 $\exp\left(\frac{ix\Xi}{\hbar}\right)$ 为动量平移算符, 其带来的动量变化为 Ξ .

□

第 4 题 (课本习题 2.2) 得分: _____. 再看一下第 1 章习题 1.11 的哈密顿量. 假定打字员出了一个错, 把 H 写成

$$H = H_{11}|1\rangle\langle 1| + H_{22}|2\rangle\langle 2| + H_{12}|1\rangle\langle 2|.$$

现在什么原理被破坏了? 通过尝试利用这类不合法的哈密顿量求解最一般的问题 (为了简单, 你可以假定 $H_{11} = H_{22} = 0$), 阐明你的观点.

解: 该非厄米的哈密顿量导致时间演化算符失去了么正性, 从而破坏了量子态在时间演化中的归一性, 即在该哈密顿量下, 量子态与自身的内积并不能总保持为 1.

简单起见, 不妨假定 $H_{11} = H_{22} = 0$, 即

$$H = H_{12}|1\rangle\langle 2|. \quad (20)$$

该不含时的哈密顿量对应的时间演化算符为

$$\begin{aligned} U(t, t_0) &= \exp\left[\frac{-iH(t-t_0)}{\hbar}\right] \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{-iH(t-t_0)}{\hbar}\right]^n \\ &\quad (\text{利用 } H^2 = H_{12}^2|1\rangle\langle 2|1\rangle\langle 2| = 0) \\ &= 1 - \frac{iH(t-t_0)}{\hbar} \end{aligned}$$

$$= 1 - \frac{iH_{12}(t-t_0)}{\hbar} |1\rangle\langle 2|. \quad (21)$$

假设 t_0 时刻的归一化量子态 $|\alpha, t_0\rangle = c_1|1\rangle + c_2|2\rangle$ 满足归一化条件 $\langle\alpha, t_0|\alpha, t_0\rangle = |c_1|^2 + |c_2|^2 = 1$, 则其演化至 t 时刻为

$$|\alpha, t_0; t\rangle = U(t, t_0)|\alpha, t_0\rangle = \left[1 - \frac{iH_{12}(t-t_0)}{\hbar} |1\rangle\langle 2|\right] (c_1|1\rangle + c_2|2\rangle) = \left[c_1 - \frac{iH_{12}(t-t_0)}{\hbar} c_2\right] |1\rangle + c_2|2\rangle. \quad (22)$$

此时量子态与自身的内积含时, 不再满足归一化条件:

$$\begin{aligned} \langle\alpha, t_0; t|\alpha, t_0; t\rangle &= \left\{ \left[c_1 + \frac{iH_{12}(t-t_0)}{\hbar} c_2 \right] \langle 1| + c_2\langle 2| \right\} \left\{ \left[c_1 - \frac{iH_{12}(t-t_0)}{\hbar} c_2 \right] |1\rangle + c_2|2\rangle \right\} \\ &= |c_1|^2 + \frac{|H_{12}|^2 (t-t_0)^2}{\hbar^2} |c_2|^2 + |c_2|^2 \\ &= 1 + \frac{|H_{12}|^2 (t-t_0)^2}{\hbar^2} |c_2|^2 \\ &\geq 1. \end{aligned} \quad (23)$$

□

第 5 题 (课本习题 2.3) 得分: _____. 一个电子受到一个时间无关的、强度为 B 的沿正 z 方向的均匀磁场的作用. 在 $t=0$ 时已知电子处在 $\mathbf{S} \cdot \hat{\mathbf{n}}$ 的本征态上, 本征值为 $\hbar/2$, 其中 $\hat{\mathbf{n}}$ 是一个单位矢量, 位于 xz 平面上, 与 z 轴夹 β 角.

- (a) 求找到电子处在 $s_x = \hbar/2$ 态上作为时间函数的概率.
- (b) 求作为时间函数的 S_x 的期待值.
- (c) 为让你自己放心, 在 (i) $\beta \rightarrow 0$ 和 (ii) $\beta \rightarrow \pi/2$ 的极端情况下证明你的答案是有意义的.

解: (a) $t=0$ 时, 电子的状态为

$$|\alpha, t=0\rangle = \cos \frac{\beta}{2} |s_z, +\rangle + \sin \frac{\beta}{2} |s_z, -\rangle. \quad (24)$$

电子和磁场相互作用的哈密顿量

$$H = -\frac{eB}{mc} S_z \equiv \omega S_z \quad (25)$$

不含时, 故对应的时间演化算符为

$$U(t, 0) = \exp\left(\frac{-iHt}{\hbar}\right) = \exp\left(\frac{-i\omega S_z t}{\hbar}\right). \quad (26)$$

t 时刻电子的状态为

$$\begin{aligned} |\alpha, t\rangle &= U(t, 0)|\alpha, t\rangle \\ &= \exp(-i\omega S_z t/\hbar) \left(\cos \frac{\beta}{2} |s_z, +\rangle + \sin \frac{\beta}{2} |s_z, -\rangle \right) \\ &= \exp(-i\omega t/2) \cos \frac{\beta}{2} |s_z, +\rangle + \exp(i\omega t/2) \sin \frac{\beta}{2} |s_z, -\rangle. \end{aligned} \quad (27)$$

电子处在 $s_x = \hbar/2$ 态上概率为

$$P(s_x = \hbar/2) = |\langle s_x = \hbar/2 | \alpha, t \rangle|^2$$

$$\begin{aligned}
&= \left| \frac{1}{\sqrt{2}} (\langle s_z, + | + \langle s_z, - |) \left[\exp(-i\omega t/2) \cos \frac{\beta}{2} |s_z, + \rangle + \exp(i\omega t/2) \sin \frac{\beta}{2} |s_z, - \rangle \right] \right|^2 \\
&= \frac{1}{2} \left| \exp(-i\omega t/2) \cos \frac{\beta}{2} + \exp(i\omega t/2) \sin \frac{\beta}{2} \right|^2 \\
&= \frac{1}{2} [1 + \sin \beta \cos(\omega t)].
\end{aligned} \tag{28}$$

(b) 算符 S_x 在基 $\{|s_z, \pm\rangle\}$ 上展开的形式为

$$S_x = \frac{\hbar}{2} (|s_z, +\rangle \langle s_z, -| + |s_z, -\rangle \langle s_z, +|). \tag{29}$$

S_x 的期待值

$$\begin{aligned}
\langle S_x(t) \rangle &= \langle \alpha, t | S_x | \alpha, t \rangle \\
&= \left[\exp(i\omega t/2) \cos \frac{\beta}{2} \langle s_z, + | + \exp(-i\omega t/2) \sin \frac{\beta}{2} \langle s_z, - | \right] \frac{\hbar}{2} (|s_z, +\rangle \langle s_z, -| + |s_z, -\rangle \langle s_z, +|) \times \\
&\quad \left[\exp(-i\omega t/2) \cos \frac{\beta}{2} |s_z, +\rangle + \exp(i\omega t/2) \sin \frac{\beta}{2} |s_z, -\rangle \right] \\
&= \frac{\hbar}{2} \sin \beta \cos(\omega t).
\end{aligned} \tag{30}$$

(c) (i) 当 $\beta = 0$, 则 $t = 0$ 时电子的状态为 $|\alpha, t = 0\rangle = |s_z, +\rangle$, 该状态为哈密顿量的本征态, 故关于时间保持不变. t 时刻电子处在 $s_x = \hbar/2$ 的概率为

$$P(s_x = \hbar/2) = |\langle s_x, + | s_z, + \rangle|^2 = \left| \frac{1}{\sqrt{2}} (\langle s_z, + | + \langle s_z, - |) |s_z, +\rangle \right|^2 = \frac{1}{2}. \tag{31}$$

这与利用 (a) 中结论得到的

$$P(s_x = \hbar/2) = \frac{1}{2} [1 + \sin 0 \cos(\omega t)] = \frac{1}{2} \tag{32}$$

一致. S_x 的期待值为

$$\langle S_x \rangle = \langle s_z, + | S_x | s_z, + \rangle = \langle s_z, + | \frac{\hbar}{2} (|s_z, +\rangle \langle s_z, -| + |s_z, -\rangle \langle s_z, +|) | s_z, + \rangle = 0. \tag{33}$$

这与利用 (b) 中结论得到的

$$\langle S_x \rangle = \frac{\hbar}{2} \sin 0 \cos(\omega t) = 0 \tag{34}$$

一致.

(ii) 当 $\beta = \pi/2$, 则 $t = 0$ 时电子的状态为

$$|\alpha, t = 0\rangle = |s_x, +\rangle = \frac{1}{\sqrt{2}} (|s_z, +\rangle + |s_z, -\rangle). \tag{35}$$

t 时刻电子的状态为

$$\begin{aligned}
|\alpha, t\rangle &= U(t, 0) |\alpha, t = 0\rangle = \exp(-i\omega S_z t/\hbar) \frac{1}{\sqrt{2}} (|s_z, +\rangle + |s_z, -\rangle) \\
&= \frac{1}{\sqrt{2}} [\exp(-i\omega t/2) |s_z, +\rangle + \exp(i\omega t/2) |s_z, -\rangle]
\end{aligned} \tag{36}$$

电子处在 $s_x = \hbar/2$ 态上的概率为

$$P(s_x = \hbar/2) = |\langle s_x = \hbar/2 | \alpha, t \rangle|^2$$

$$\begin{aligned}
&= \left| \frac{1}{\sqrt{2}} (\langle s_z, + | + \langle s_z, - |) \frac{1}{\sqrt{2}} [\exp(-i\omega t/2) |s_z, + \rangle + \exp(i\omega t/2) |s_z, - \rangle] \right|^2 \\
&= \cos^2(\omega t/2).
\end{aligned} \tag{37}$$

这与利用 (a) 中结论得到的

$$P(s_x = \hbar/2) = \frac{1}{2} \left[1 + \sin \frac{\pi}{2} \cos(\omega t) \right] = \cos^2(\omega t/2) \tag{38}$$

一致. S_x 的期待值为

$$\begin{aligned}
\langle S_x \rangle &= \langle \alpha, t | S_x | \alpha, t \rangle \\
&= \frac{1}{\sqrt{2}} [\exp(i\omega t/2) \langle s_z, + | + \exp(-i\omega t/2) \langle s_z, - |] \frac{\hbar}{2} (|s_z, + \rangle \langle s_z, - | + |s_z, - \rangle \langle s_z, + |) \times \\
&\quad \frac{1}{\sqrt{2}} [\exp(-i\omega t/2) |s_z, + \rangle + \exp(i\omega t/2) |s_z, - \rangle] \\
&= \frac{\hbar}{2} \cos(\omega t).
\end{aligned} \tag{39}$$

这与利用 (b) 中结论得到的

$$\langle S_x \rangle = \frac{\hbar}{2} \sin \frac{\pi}{2} \cos(\omega t) = \frac{\hbar}{2} \cos(\omega t) \tag{40}$$

一致.

综上, (a) 和 (b) 中得到的结论应当是可靠的.

□

第 6 题 (课本习题 2.6) 得分: _____. 考虑一个一维粒子, 其哈密顿量由下式给出

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

通过计算 $[[H, x], x]$, 证明

$$\sum_{a'} |\langle a'' | x | a' \rangle|^2 (E_{a'} - E_{a''}) = \frac{\hbar^2}{2m},$$

其中 $|a'\rangle$ 是一个能量本征态, 本征值为 $E_{a'}$.

证:

$$[H, x] = \left[\frac{p^2}{2m} + V(x), x \right] = \left[\frac{p^2}{2m}, x \right] + [V(x), x] = \frac{1}{2m} [p^2, x] = \frac{1}{2m} (p[p, x] + [p, x]p) = -i \frac{\hbar}{m} p. \tag{41}$$

$$[[H, x], x] = \left[-i \frac{\hbar}{m} p, x \right] = -\frac{\hbar^2}{m}. \tag{42}$$

一方面,

$$\begin{aligned}
\sum_{a'} |\langle a'' | x | a' \rangle|^2 (E_{a'} - E_{a''}) &= \sum_{a'} [\langle a'' | x | a' \rangle E_{a'} \langle a' | x | a'' \rangle - \langle a'' | x | a' \rangle E_{a''} \langle a' | x | a'' \rangle] \\
&= \sum_{a'} [\langle a'' | x H | a' \rangle \langle a' | x | a'' \rangle - \langle a'' | H x | a' \rangle \langle a' | x | a'' \rangle] \\
&= \sum_{a'} \langle a'' | (xH - Hx) | a' \rangle \langle a' | x | a'' \rangle \\
&= \langle a'' | [x, H] x | a'' \rangle,
\end{aligned} \tag{43}$$

另一方面,

$$\begin{aligned}
 \sum_{a'} |\langle a'' | x | a' \rangle|^2 (E_{a'} - E_{a''}) &= \sum_{a'} [\langle a'' | x | a' \rangle E_{a'} \langle a' | x | a'' \rangle - \langle a'' | x | a' \rangle E_{a''} \langle a' | x | a'' \rangle] \\
 &= \sum_{a'} [\langle a'' | x | a' \rangle \langle a' | H x | a'' \rangle - \langle a'' | x | a' \rangle \langle a' | x H | a'' \rangle] \\
 &= \sum_{a'} \langle a'' | x | a' \rangle \langle a' | (H x - x H) | a'' \rangle \\
 &= \langle a'' | x [H, x] | a'' \rangle.
 \end{aligned} \tag{44}$$

以上两式相加得

$$\begin{aligned}
 2 \sum_{a'} |\langle a'' | x | a' \rangle|^2 (E_{a'} - E_{a''}) &= \langle a'' | [x, H] x | a'' \rangle + \langle a'' | x [H, x] | a'' \rangle \\
 &= - \langle a'' | ([H, x] x - x [H, x]) | a'' \rangle \\
 &= - \langle a'' | [[H, x], x] | a'' \rangle \\
 &= \frac{\hbar^2}{m},
 \end{aligned} \tag{45}$$

$$\Rightarrow \sum_{a'} |\langle a'' | x | a' \rangle|^2 (E_{a'} - E_{a''}) = \frac{\hbar^2}{2m}. \tag{46}$$

□

第 7 题 (课本习题 2.8) 得分: _____. 考虑一个一维自由粒子的波包. $t = 0$ 时它满足最小不确定度关系

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \frac{\hbar^2}{4} \quad (t = 0).$$

此外, 我们知道

$$\langle x \rangle = \langle p \rangle = 0 \quad (t = 0).$$

利用海森堡绘景, 当 $\langle (\Delta x)^2 \rangle_{t=0}$ 给定时, 求作为 t ($t \geq 0$) 的函数的 $\langle (\Delta x)^2 \rangle_t$. (提示: 利用你在第 1 章习题 1.18 中得到的不确定度波包的性质.)

解: 一维自由粒子的哈密顿量为

$$H = \frac{p^2}{2m}. \tag{47}$$

对应的时间演化算符为

$$U(t, 0) = \exp \left(\frac{-ip^2 t}{2m\hbar} \right). \tag{48}$$

从而

$$\begin{aligned}
 \langle (\Delta x)^2 \rangle_t &= \langle x^2 \rangle_t - \langle x \rangle_t^2 \\
 &= \langle \alpha, t = 0 | U^\dagger(t, 0) x^2 U(t, 0) | \alpha, t = 0 \rangle - \langle \alpha, t = 0 | U^\dagger(t, 0) x U(t, 0) | \alpha, t = 0 \rangle^2.
 \end{aligned} \tag{49}$$

利用 Baker-Campbell-Hausdorff 公式 $e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!} [X, [X, Y]] + \frac{1}{3!} [X, [X, [X, Y]]] + \dots$, 有

$$\begin{aligned}
 U^\dagger(t, 0) x^2 U(t, 0) &= \exp \left(\frac{ip^2 t}{2m} \right) x^2 \exp \left(\frac{-ip^2 t}{2m} \right) \\
 &= x^2 + \left[\frac{ip^2 t}{2m}, x^2 \right] + \frac{1}{2!} \left[\frac{ip^2 t}{2m}, \left[\frac{ip^2 t}{2m}, x^2 \right] \right] + \frac{1}{3!} \left[\frac{ip^2 t}{2m}, \left[\frac{ip^2 t}{2m}, \left[\frac{ip^2 t}{2m}, x^2 \right] \right] \right] + \dots
 \end{aligned}$$

$$=x^2 + \frac{t}{m}(px + xp) + \left(\frac{t}{m}\right)^2 p^2, \quad (50)$$

$$\begin{aligned} U^\dagger(t, 0)xU(t, 0) &= \exp\left(\frac{ip^2t}{2m}\right)x\exp\left(\frac{-ip^2t}{2m}\right) \\ &= x + \left[\frac{ip^2t}{2m}, x\right] + \frac{1}{2!}\left[\frac{ip^2t}{2m}, \left[\frac{ip^2t}{2m}, x\right]\right] + \frac{1}{3!}\left[\frac{ip^2t}{2m}, \left[\frac{ip^2t}{2m}, \left[\frac{ip^2t}{2m}, x\right]\right]\right] + \cdots \\ &= x + \frac{t}{m}p. \end{aligned} \quad (51)$$

故

$$\begin{aligned} \langle(\Delta x)^2\rangle_t &= \langle\alpha, t=0|\left[x^2 + \frac{t}{m}(px + xp) + \left(\frac{t}{m}\right)^2 p^2\right]|\alpha, t=0\rangle - \langle\alpha, t=0|\left(x + \frac{t}{m}p\right)|\alpha, t=0\rangle^2 \\ &= \langle x^2\rangle_{t=0} + \frac{t}{m}\langle px + xp\rangle_{t=0} + \left(\frac{t}{m}\right)^2 \langle p^2\rangle_{t=0} - \left[\langle x\rangle_{t=0} + \frac{t}{m}\langle p\rangle_{t=0}\right]^2 \\ &= \langle x^2\rangle_{t=0} + \frac{t}{m}\langle px + xp\rangle_{t=0} + \left(\frac{t}{m}\right)^2 \langle p^2\rangle_{t=0}. \end{aligned} \quad (52)$$

由于该粒子在 $t=0$ 时满足最小不确定度关系, 有

$$\langle p^2\rangle_{t=0} = \langle(p - \langle p\rangle_{t=0})^2\rangle = \langle(\Delta p)^2\rangle = \frac{\hbar^2}{4} \frac{1}{\langle(\Delta x)^2\rangle_{t=0}}. \quad (53)$$

及

$$\langle(\Delta x)^2\rangle_{t=0}\langle(\Delta p)^2\rangle_{t=0} = \frac{1}{4} |\langle[\Delta x, \Delta p]\rangle_{t=0}|^2 + \frac{1}{4} |\langle\{\Delta x, \Delta p\}\rangle_{t=0}|^2 = \frac{\hbar^2}{4} + \frac{1}{4} |\langle\{\Delta x, \Delta p\}\rangle_{t=0}|^2 = \frac{\hbar^2}{4}, \quad (54)$$

$$\implies \langle\{\Delta x, \Delta p\}\rangle_{t=0} = \langle xp + px\rangle_{t=0} = 0. \quad (55)$$

故

$$\langle(\Delta x)^2\rangle_t = \langle(\Delta x)^2\rangle_{t=0} + \frac{\hbar^2 t^2}{4m^2} \frac{1}{\langle(\Delta x)^2\rangle_{t=0}}. \quad (56)$$

□