高等量子力学第三次作业

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习题 1.21

在相干态表象下求 $\hat{a}$ 和 $\hat{a}^\dagger\hat{a}$ 的本征值和本征态。

可以计算:

$$\hat{a}\left|\bar{\alpha}\right\rangle=\sum_{n=1}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\hat{a}\left|n\right\rangle+\hat{a}\left|0\right\rangle=\alpha\sum_{n=1}^{\infty}\frac{\alpha^{n-1}}{\sqrt{(n-1)!}}\left|n-1\right\rangle=\alpha\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\left|n\right\rangle=\alpha\left|\bar{\alpha}\right\rangle.$$

将 $\hat{a}^\dagger\hat{a}$ 本征态记作 $|\psi\rangle$，本征值记作 λ，在相干态表象下本征值方程为:

$$\langle\bar{\alpha}|\,\hat{a}^\dagger\hat{a}\,|\psi\rangle=\alpha^*\frac{\partial}{\partial\alpha^*}\langle\bar{\alpha}|\,\psi\rangle=\lambda\langle\bar{\alpha}|\,\psi\rangle.$$

不难注意到，当 $\langle\bar{\alpha}|\,\psi\rangle=c_n(\alpha^*)^n$ 时，上述本征值方程为:

$$\alpha^*\frac{\partial}{\partial\alpha^*}c_n(\alpha^*)^n=nc_n(\alpha^*)^n=\lambda c_n(\alpha^*)^n.$$

即 $\lambda=n$，由归一化条件 $\langle\psi|\,\psi\rangle=\int d\mu(\alpha)\langle\psi|\,\bar{\alpha}\rangle\langle\bar{\alpha}|\,\psi\rangle=1$ 可以计算 $c_n=\frac{1}{\sqrt{n!}}$，即 $\hat{a}^\dagger\hat{a}$ 的本征态 $|\psi\rangle$ 满足 $\langle\bar{\alpha}|\,\psi\rangle=\frac{(\alpha^*)^n}{\sqrt{n!}}$ 本征值为 n。

注意到 $\langle\bar{\alpha}|=\sum_n\frac{(\alpha^*)^n}{\sqrt{n!}}\langle n|$，则 $\hat{a}^\dagger\hat{a}$ 的本征态为 $|\psi\rangle=|n\rangle$。

习题 1.22

证明任意密度矩阵算符满足

$$\mathbf{Tr}(\hat{\rho}^2)\leq 1.$$

当且仅当

$$\mathbf{Tr}(\hat{\rho}^2)=1.$$

体系处于纯态。

对于任意密度矩阵算符 $\hat{\rho}=\sum_i p_i\left|\psi_i\right\rangle\left\langle\psi_i\right|$，可以计算:

$$\hat{\rho}^2=\sum_{i,j}p_ip_j\left|\psi_i\right\rangle\langle\psi_i|\,\psi_j\rangle\left\langle\psi_j\right|.$$

则可以计算:

$$\mathbf{Tr}(\hat{\rho}^2)=\sum_{i,j}p_ip_j\langle\psi_j|\,\psi_i\rangle\langle\psi_i|\,\psi_j\rangle=\sum_{i,j}p_ip_j|\langle\psi_i|\,\psi_j\rangle|^2\leq\sum_{i,j}p_ip_j=\left(\sum_i p_i\right)\left(\sum_j p_j\right)=1.$$

对于纯态，密度矩阵算符可以写作 $\hat{\rho}=|\psi\rangle\langle\psi|$，则容易计算:

$$\mathbf{Tr}(\hat{\rho}^2)=\mathbf{Tr}(\hat{\rho})=1.$$

对于任意密度矩阵算符 $\hat{\rho}=\sum_i p_i \left|\psi_i\right\rangle\left\langle\psi_i\right|$，因为其为厄米算符，所以总可以选取一个表象，使得密度矩阵算符对角化，记作 $\hat{\rho}=\sum_j p'_j \left|\phi_j\right\rangle\left\langle\phi_j\right|$，其中 $\left\langle\phi_i\middle|\phi_j\right\rangle=\delta_{ij}$。则可以计算：

$$\mathbf{Tr}(\hat{\rho}^2)=\sum_{i,j}p'_ip'_j|\left\langle\phi_i\middle|\phi_j\right\rangle|^2=\sum_i p_i'^2\leq\left(\sum_i p'_i\right)^2=1.$$

等号成立的条件为只存在唯一一个 $p'=1$。即此时密度矩阵算符为：

$$\hat{\rho}=\left|\phi\right\rangle\left\langle\phi\right|.$$

即体系处于纯态。

综上所述，密度矩阵算符满足 $\mathbf{Tr}(\hat{\rho}^2)\leq 1$，当且仅当 $\mathbf{Tr}(\hat{\rho}^2)=1$ 时体系处于纯态。

习题 **1.23**

证明二能级系统的密度算符矩阵可以写作

$$\hat{\rho}=\frac{\mathbf{I}+\vec{r}\cdot\vec{\sigma}}{2}$$

其中 $\vec{\sigma}=\sigma_x\vec{e}_x+\sigma_y\vec{e}_y+\sigma_z\vec{e}_z$，$\sigma_x,\sigma_y,\sigma_z$ 为 Pauli 矩阵，$\vec{e}_x,\vec{e}_y,\vec{e}_z$ 为 x,y,z 方向的单位矢量。矢量 $\vec{r}$ 满足：

$$|\vec{r}|=r\leq 1.$$

当且仅当 $r=1$ 时，体系处于纯态。

二能级系统的密度算符矩阵可以写作：

$$\hat{\rho}=p\left|\psi_1\right\rangle\left\langle\psi_1\right|+(1-p)\left|\psi_2\right\rangle\left\langle\psi_2\right|.$$

考虑这个算符在 $\{\left|u_1\right\rangle,\left|u_2\right\rangle\}$ 表象下的矩阵元可以计算得：

$$\begin{aligned}
\left\langle u_1\right|\hat{\rho}\left|u_1\right\rangle=&p\alpha_1\alpha_1^*+(1-p)\beta_1\beta_1^*;\\
\left\langle u_1\right|\hat{\rho}\left|u_2\right\rangle=&p\alpha_1\alpha_2^*+(1-p)\beta_1\beta_2^*;\\
\left\langle u_2\right|\hat{\rho}\left|u_1\right\rangle=&p\alpha_2\alpha_1^*+(1-p)\beta_2\beta_1^*;\\
\left\langle u_2\right|\hat{\rho}\left|u_2\right\rangle=&p\alpha_2\alpha_2^*+(1-p)\beta_2\beta_2^*.
\end{aligned}$$

其中：

$$\alpha_1=\left\langle u_1\middle|\psi_1\right\rangle,\ \alpha_2=\left\langle u_2\middle|\psi_1\right\rangle,\ \beta_1=\left\langle u_1\middle|\psi_2\right\rangle,\ \beta_2=\left\langle u_2\middle|\psi_2\right\rangle.$$

则不难注意到：

$$|\alpha_1|^2+|\alpha_2|^2=1,\ |\beta_1|^2+|\beta_2|^2=1,\ |\alpha_1|^2+|\beta_1|^2=1,\ |\alpha_2|^2+|\beta_2|^2=1.$$

可以计算：

$$\left\langle u_1\right|\hat{\rho}\left|u_1\right\rangle+\left\langle u_2\right|\hat{\rho}\left|u_2\right\rangle=1.$$

同时，令：

$$x=\left\langle u_1\right|\hat{\rho}\left|u_2\right\rangle+\left\langle u_2\right|\hat{\rho}\left|u_1\right\rangle=p(\alpha_1\alpha_2^*+\alpha_2\alpha_1^*)+(1-p)(\beta_1\beta_2^*+\beta_2\beta_1^*);$$

$$iy = \langle u_1 | \hat{\rho} | u_2 \rangle - \langle u_2 | \hat{\rho} | u_1 \rangle = p(\alpha_1 \alpha_2^* - \alpha_2 \alpha_1^*) + (1-p)(\beta_1 \beta_2^* - \beta_2 \beta_1^*);$$
$$z = \langle u_1 | \hat{\rho} | u_1 \rangle - \langle u_2 | \hat{\rho} | u_2 \rangle = p(\alpha_1 \alpha_1^* - \alpha_2 \alpha_2^*) + (1-p)(\beta_1 \beta_1^* - \beta_2 \beta_2^*).$$

则密度矩阵算符的矩阵表示可以写作:

$$\rho = \begin{pmatrix} \frac{1}{2} + \frac{z}{2} & \frac{x}{2} + \frac{iy}{2} \\ \frac{x}{2} - \frac{iy}{2} & \frac{1}{2} - \frac{z}{2} \end{pmatrix} = \frac{\mathbf{I} + \vec{r} \cdot \vec{\sigma}}{2}$$

可以计算:

$$\begin{aligned} |\vec{r}|^2 =& |x|^2 + |y|^2 + |z|^2 \\ =& p^2 + (1-p)^2 + 2p(1-p)(4\mathbf{Re}(\alpha_1 \alpha_2^* \beta_1^* \beta_2) - (1 - 2|\alpha_1|^2)^2) \\ \leq& p^2 + (1-p)^2 + 2p(1-p)(4|\alpha_1|^2 - 4|\alpha_1|^4 - (1-2|\alpha_1|^2)^2) \\ =& p^2 + (1-p)^2 + 2p(1-p) - 4p(1-p)(2|\alpha_1|^2 - 1)^2 \\ =& 1 - 4p(1-p)(2|\alpha_1|^2 - 1)^2 \\ \leq& 1. \end{aligned}$$

则有:

$$|\vec{r}| = r \leq 1.$$

当 $r = 1$ 时，有: $p = 0$ 或 $p = 1$，显然此时有 $\hat{\rho}^2 = \hat{\rho}$，体系处于纯态。
当体系处于纯态时，有 $\hat{\rho}^2 = \hat{\rho}$，则可以计算:

$$\begin{aligned} \hat{\rho}^2 =& \frac{1}{4}(\mathbf{I} + \vec{r} \cdot \vec{\sigma})^2 \\ =& \frac{1}{4}(\mathbf{I} + 2\vec{r} \cdot \vec{\sigma} + (\vec{r} \cdot \vec{\sigma})^2) \\ =& \frac{1}{4}((1 + r^2)\mathbf{I} + 2\vec{r} \cdot \vec{\sigma}) \\ =& \hat{\rho}. \end{aligned}$$

则有 $|\vec{r}| = r = 1$。
综上所述，二能级系统的密度算符矩阵可以写作:

$$\hat{\rho} = \frac{\mathbf{I} + \vec{r} \cdot \vec{\sigma}}{2}$$

当且仅当 $r = 1$ 时，体系处于纯态。

习题 1.24

证明 $\hat{\rho}_1 = \mathbf{Tr}_2(|\psi\rangle_{12}\,{}_{12}\langle\psi|)$ 为密度矩阵算符，并且 $\hat{\rho}_1$ 为纯态的充要条件为 $|\psi\rangle_{12}$ 为直积态。

可以计算:

$$\mathbf{Tr}(\hat{\rho}_1) = \mathbf{Tr}_1(\mathbf{Tr}_2(|\psi\rangle_{12}\,{}_{12}\langle\psi|)) = \mathbf{Tr}_{12}(|\psi\rangle_{12}\,{}_{12}\langle\psi|) = 1.$$
$$\hat{\rho}_1^\dagger = [\mathbf{Tr}_2(|\psi\rangle_{12}\,{}_{12}\langle\psi|)]^\dagger = \mathbf{Tr}_2(|\psi\rangle_{12}\,{}_{12}\langle\psi|) = \hat{\rho}_1$$

对于任意态矢量 $|a\rangle = \sum \alpha_m |m\rangle$，可以计算:

$$
\begin{aligned}
\langle a|\hat{\rho}_1|a\rangle =& \langle a|\mathbf{Tr}_2(|\psi\rangle_{12\,12}\langle\psi|)|a\rangle \\
=&\mathbf{Tr}_1(|a\rangle\langle a|\mathbf{Tr}_2(|\psi\rangle_{12\,12}\langle\psi|)) \\
=&\mathbf{Tr}_{12}(|a\rangle\langle a|\otimes\mathbf{1}_2)(|\psi\rangle_{12\,12}\langle\psi|) \\
=&_{12}\langle\psi|(|a\rangle\langle a|\otimes\mathbf{1}_2)|\psi\rangle_{12} \\
=&\sum_{m,n} c^*_{mn\,1}\langle m|\otimes{}_2\langle n|(|a\rangle\langle a|\otimes\mathbf{1}_2)\sum_{m',n'} c_{m'n'}|m'\rangle_1\otimes|n'\rangle_2 \\
=&\sum_{m,m',n} c^*_{mn}c_{m'n}\langle m|a\rangle\langle a|m'\rangle \\
=&\sum_n\left(\sum_m c^*_{mn}\langle m|a\rangle\right)\left(\sum_m c_{mn}\langle a|m\rangle\right) \\
\geq&0.
\end{aligned}
$$

若 $|\psi\rangle_{12} = |\phi\rangle_1\otimes|\chi\rangle_2$，则有:

$$
\hat{\rho}_1 = \mathbf{Tr}_2(|\psi\rangle_{12\,12}\langle\psi|) = {}_2\langle\chi|\chi\rangle_2|\phi\rangle_{1\,1}\langle\phi| = |\phi\rangle_{1\,1}\langle\phi| = |\phi\rangle\langle\phi|.
$$

则有:

$$
\hat{\rho}_1^2 = |\phi\rangle\langle\phi|\phi\rangle\langle\phi| = |\phi\rangle\langle\phi| = \hat{\rho}_1.
$$

若 $\hat{\rho}_1$ 为纯态，即 $\hat{\rho}_1^2 = \hat{\rho}_1$。可以计算:

$$
\begin{aligned}
\hat{\rho}_1 =&\mathbf{Tr}_2(\sum_{m,n} c_{mn}|m\rangle\otimes|n\rangle\sum_{m',n'} c^*_{m'n'}\langle m'|\langle n'|) \\
=&\sum_{m,n,m',n'} c_{mn}c^*_{m'n'}|m\rangle\langle m'|\langle n'|n\rangle \\
=&\sum_{m,m',n} c_{mn}c^*_{m',n}|m\rangle\langle m'| \\
\hat{\rho}_1^2 =&\sum_{m_1,m_2,m_3,m_4,n_1,n_2} c_{m_1,n_1}c^*_{m_2,n_1}c_{m_3,n_2}c^*_{m_4,n_2}|m_1\rangle\langle m_2|m_3\rangle\langle m_4| \\
=&\sum_{m,m',n} c_{mn}c^*_{m'n}|m\rangle\langle m'| = \hat{\rho}_1
\end{aligned}
$$

当且仅当满足 $c_{mn} = \alpha_m\beta_n$ 时上式成立。此时可以计算:

$$
\begin{aligned}
\hat{\rho}_1 =&\mathbf{Tr}_2(\sum_{m,n}\alpha_m\beta_n|m\rangle\otimes|n\rangle\sum_{m',n'}\alpha^*_{m'}\beta^*_{n'}\langle m'|\langle n'|) \\
=&\sum_{m,n,m',n'}\alpha_m\beta_n\alpha^*_m\beta^*_n|m\rangle\langle m'|\langle n'|n\rangle \\
=&\sum_{m,m'}\alpha_m\alpha^*_{m'}|m\rangle\langle m'|
\end{aligned}
$$

$$\begin{aligned}\hat{\rho}_1^2 &= \sum_{m_1,m_2,m_3,m_4} \alpha_{m_1}\alpha_{m_2}^*\alpha_{m_3}\alpha_{m_4}^* |m_1\rangle \langle m_2| m_3\rangle \langle m_4| \\ &= \sum_{m,m'} \alpha_m \alpha_{m'}^* |m\rangle \langle m'| .\end{aligned}$$

当 $c_{mn} = \alpha_m\beta_n$ 时，则有:

$$|\psi\rangle = \sum_{mn} \alpha_m\beta_n |m\rangle \otimes |n\rangle = \left(\sum_m \alpha_m |m\rangle\right) \otimes \left(\sum_n \beta_n |n\rangle\right).$$

即 $|\psi\rangle_{12}$ 可以写作直积态。

综上所述，$\hat{\rho}_1$ 为纯态的充要条件为 $|\psi\rangle_{12}$ 为直积态。

习题 1.25

证明对于量子态

$$|B\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

可以选择 $\vec{n}_1, \vec{n}_2, \vec{n}_3, \vec{n}_4$，使得 $|\langle \hat{B}\rangle| = 2\sqrt{2}$

选取四个向量分别为:

$$\begin{aligned}\vec{n}_1 &= (1/\sqrt{2} \quad 0 \quad 1/\sqrt{2}); & \vec{n}_2 &= (1 \quad 0 \quad 0); \\ \vec{n}_3 &= (1/\sqrt{2} \quad 0 \quad -1/\sqrt{2}); & \vec{n}_4 &= (0 \quad 0 \quad 1).\end{aligned}$$

可以计算:

$$\begin{aligned}\vec{\sigma}_1 \cdot \vec{n}_1 &= \frac{1}{\sqrt{2}}\sigma_x + \frac{1}{\sqrt{2}}\sigma_z = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}; \\ \vec{\sigma}_2 \cdot (\vec{n}_2 + \vec{n}_4) &= \sigma_x + \sigma_z = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}; \\ \vec{\sigma}_1 \cdot \vec{n}_3 &= \frac{1}{\sqrt{2}}\sigma_x - \frac{1}{\sqrt{2}}\sigma_z = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}; \\ \vec{\sigma}_2 \cdot (\vec{n}_2 - \vec{n}_4) &= \sigma_x - \sigma_z = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.\end{aligned}$$

则可以计算:

$$\hat{B} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \sqrt{2} & 0 & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & \sqrt{2} & 0 \\ 0 & \sqrt{2} & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 & \sqrt{2} \end{pmatrix}.$$

则可以计算:

$$\langle B|\,\hat{B}\,|B\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & \sqrt{2} & 0 \\ 0 & \sqrt{2} & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 & \sqrt{2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = 2\sqrt{2}.$$

习题 1.26

证明

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathbf{Tr}(e^{-\beta\hat{H}})}$$

为密度算符。其中 $\beta = k_B T$，k_B 为玻尔兹曼常数，T 为温度。

因为 $\hat{H}^\dagger = \hat{H}$，则有:

$$\hat{\rho}^\dagger = \frac{1}{\mathbf{Tr}(e^{-\beta\hat{H}})}\left(\sum_{n=0}^{\infty}\frac{(-\beta\hat{H})^n}{n!}\right)^\dagger = \frac{1}{\mathbf{Tr}(e^{-\beta\hat{H}})}\left(\sum_{n=0}^{\infty}\frac{(-\beta\hat{H})^n}{n!}\right) = \frac{e^{-\beta\hat{H}}}{\mathbf{Tr}(e^{-\beta\hat{H}})} = \hat{\rho}.$$

可以计算:

$$\mathbf{Tr}(\hat{\rho}) = \frac{\mathbf{Tr}(e^{-\beta\hat{H}})}{\mathbf{Tr}(e^{-\beta\hat{H}})} = 1.$$

由于指数函数的正定性，即对于任意量子态 $|\psi\rangle$，都有:

$$\langle\psi|\,e^{-\beta\hat{H}}\,|\psi\rangle > 0.$$

则有 $\hat{\rho} \geq 0$.

综上所述，$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathbf{Tr}(e^{-\beta\hat{H}})}$ 为密度算符。

习题 1.27

证明下列关系式:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + \frac{1}{1!}[\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \cdots$$

如果算符 $\hat{A}$ 存在对角化

$$\hat{A} = \sum_a |a\rangle\, a\, \langle a|$$

其中 $\langle a|\,a'\rangle = \delta_{a,a'}$，那么我们定义对任意函数 $f(x)$

$$f(\hat{A}) = \sum_a |a\rangle\, f(a)\, \langle a|$$

可以证明当函数 $f(x)$ 可泰勒展开时，上述定义与定义 (1.210) 一致。

对于在区域 D 上解析的函数 $f(z)$，如果算符 $\hat{A}$ 的本征值在 D 内，那么算符函数

$$f(\hat{A}) = \frac{1}{2\pi i}\int_\Gamma dz f(z)\frac{1}{z-A}$$

其中 Γ 为区域 D 中包含所有 $\hat{A}$ 的本征值的任意正向闭合路径。可以证明该定义与定义 (1.225) 的一致性。

$$(\hat{A}\hat{B})^{-1}=\hat{B}^{-1}\hat{A}^{-1},\quad (\hat{A}+\hat{B})^{-1}=\hat{A}^{-1}-\hat{A}^{-1}\hat{B}(\hat{A}+\hat{B})^{-1}$$

对于 $e^{\hat{A}}$ 进行 Taylor 展开有:

$$e^{\hat{A}}=\sum_{n=0}^{\infty}\frac{1}{n!}\hat{A}^n=\left(1+\hat{A}+\frac{1}{2!}\hat{A}^2+\cdots\right).$$

则展开 $e^{\hat{A}}\hat{B}e^{-\hat{A}}$，可得:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}}=\left(1+\hat{A}+\frac{1}{2!}\hat{A}^2+\cdots\right)\hat{B}\left(1-\hat{A}+\frac{1}{2!}\hat{A}^2+\cdots\right).$$

其中，可以计算 $\hat{A}$ 的零阶项为 $\hat{B}$，$\hat{A}$ 的一阶项为 $\hat{A}\hat{B}-\hat{B}\hat{A}=[\hat{A},\hat{B}]$，$\hat{A}$ 的二阶项为 $\frac{1}{2!}\hat{A}^2\hat{B}-\hat{A}\hat{B}\hat{A}+\frac{1}{2!}\hat{B}\hat{A}^2=\frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]$，以此类推，可得:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}}=\hat{B}+\frac{1}{1!}[\hat{A},\hat{B}]+\frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]+\cdots$$

可以计算:

$$\hat{A}^n=\sum_{a_1,a_2,\ldots,a_n}\prod_{i=1}^{n}a_i\left|a_1\right\rangle\left\langle a_1\right|a_2\rangle\left\langle a_2\right|\cdots\left|a_n\right\rangle\left\langle a_n\right|=\sum_a a^n\left|a\right\rangle\left\langle a\right|.$$

则有:

$$\begin{aligned}f(\hat{A})&=\sum_{n=0}^{\infty}\frac{1}{n!}f^{(n)}(0)\hat{A}^n=\sum_{n=0}^{\infty}\frac{1}{n!}f^{(n)}(0)\sum_a a^n\left|a\right\rangle\left\langle a\right|\\&=\sum_a\left|a\right\rangle\sum_{n=0}^{\infty}\frac{1}{n!}f^{(n)}(0)a^n\left\langle a\right|=\sum_a\left|a\right\rangle f(a)\left\langle a\right|.\end{aligned}$$

令 $g(\hat{A})=\frac{1}{z-\hat{A}}$，则有:

$$g(\hat{A})=\sum_a\left|a\right\rangle g(a)\left\langle a\right|=\sum_a\left|a\right\rangle\frac{1}{z-a}\left\langle a\right|.$$

从而可以计算算符函数:

$$f(\hat{A})=\frac{1}{2\pi i}\int_\Gamma dzf(z)g(\hat{A})=\frac{1}{2\pi i}\sum_a\left|a\right\rangle\int_\Gamma dzf(z)\frac{1}{z-a}\left\langle a\right|=\sum_a\left|a\right\rangle f(a)\left\langle a\right|.$$

可以计算:

$$(\hat{A}\hat{B})^{-1}(\hat{A}\hat{B})=\hat{B}^{-1}\hat{A}^{-1}\hat{A}\hat{B}=\hat{B}^{-1}\hat{B}=\mathbf{1}.$$

$$(\hat{A}+\hat{B})^{-1}(\hat{A}+\hat{B})=(\hat{A}^{-1}-\hat{A}^{-1}\hat{B}(\hat{A}+\hat{B})^{-1})(\hat{A}+\hat{B})=\mathbf{1}+\hat{A}^{-1}\hat{B}-\hat{A}^{-1}\hat{B}=\mathbf{1}.$$

其中利用了 $(\hat{A}+\hat{B})^{-1}(\hat{A}+\hat{B})=\mathbf{1}$。

综上所述，有:

$$(\hat{A}\hat{B})^{-1}=\hat{B}^{-1}\hat{A}^{-1},\quad (\hat{A}+\hat{B})^{-1}=\hat{A}^{-1}-\hat{A}^{-1}\hat{B}(\hat{A}+\hat{B})^{-1}.$$