0.1　量子计算基础

0.1.1　量子纠缠

0.1.1.1　双量子比特态

量子比特有两种状态 $|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ 和 $|\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. 通过张量积规则 $\begin{pmatrix}a_1\\a_2\end{pmatrix} \otimes \begin{pmatrix}b_1\\b_2\end{pmatrix} = \begin{pmatrix}a_1\begin{pmatrix}b_1\\b_2\end{pmatrix}\\a_2\begin{pmatrix}b_1\\b_2\end{pmatrix}\end{pmatrix} = \begin{pmatrix}a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2\end{pmatrix}$ 计算复合系统的基矢 $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$. 所以双量子比特 Hilbert 空间中的态可以展开为基矢的线性组合:

$$|\psi\rangle = \psi_1|\uparrow\uparrow\rangle + \psi_2|\uparrow\downarrow\rangle + \psi_3|\downarrow\uparrow\rangle + \psi_4|\downarrow\downarrow\rangle = \begin{pmatrix}\psi_1\\\psi_2\\\psi_3\\\psi_4\end{pmatrix}$$

0.1.1.2　双量子比特算符

通过 Pauli 矩阵约定 $\sigma_0 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$, $\sigma^{1,2,3} = \sigma^{x,y,z}$, 且其张量积积简写为 $\sigma_A^i \otimes \sigma_B^j \equiv \sigma^{ij}$, 矩阵张量积规则为

$$\sigma^{32} = \begin{pmatrix}1&0\\0&-1\end{pmatrix} \otimes \sigma^2 = \begin{pmatrix}1\sigma^2&0\sigma^2\\0\sigma^2&-1\sigma^2\end{pmatrix} = \begin{pmatrix} & -i & & \\ i & & & \\ & & & i \\ & & -i & \end{pmatrix}$$

这相当于是在给定算符的 ”基”. 即观测量矩阵都可以展开为这些矩阵张量积的线性组合. 谈论单量子比特的观测量时, 相当于默认另一个量子比特算符为 $\mathbb{I} = \sigma^0$, 使得算符基为 $(\sigma^{10}, \sigma^{20}, \sigma^{30})$ 和 $(\sigma^{01}, \sigma^{02}, \sigma^{03})$.

0.1.1.3　双量子比特模型

双量子比特 Heisenberg 模型哈密顿量为 $H = \frac{J}{4}\vec{\sigma}_A \cdot \vec{\sigma}_B$, 将其写作矩阵形式:

$$H = \frac{J}{4}(\sigma^{11} + \sigma^{22} + \sigma^{33}) = \frac{J}{4}\begin{pmatrix}1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1\end{pmatrix}$$

将其对角化以计算本征值, 并找到本征值对应的本征态, 结果为

$$E_s = -\frac{3}{4}J, \quad |s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad \text{自旋单态}$$

$$E_t = \frac{J}{4}, \quad \begin{cases} |t_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |t_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \\ |t_3\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \end{cases}, \quad \text{自旋三重态}$$

0.1.1.4　自旋单态

$$|s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}, \vec{\sigma}_A = (\sigma^{10}, \sigma^{20}, \sigma^{30}) = \left(\begin{pmatrix} & & 1 & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{pmatrix}, \begin{pmatrix} & & -i & \\ & & & -i \\ i & & & \\ & i & & \end{pmatrix}, \begin{pmatrix}1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1\end{pmatrix}\right)$$

0.1.1.5　纠缠熵

双量子比特态 $|\psi\rangle$ 中量子比特 A 的纠缠熵: $S(A) = -\text{Tr}[\rho_A \ln \rho_A]$. 其中约化密度矩阵 $\rho_A = \text{Tr}_B|\psi\rangle\langle\psi|$
更广义的 Renyi 纠缠熵 $S^{(n)}(A) = \dfrac{1}{1-n}\ln \text{Tr}\rho_A^n$.
接下来介绍如何部分求迹.

1. 自旋单态 $|\psi\rangle = |s\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. 其总密度矩阵为

$$\rho = |s\rangle\langle s| = \frac{1}{2}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\begin{pmatrix}0 & 1 & -1 & 0\end{pmatrix} = \frac{1}{2}\begin{pmatrix} & & & \\ & 1 & -1 & \\ & -1 & 1 & \\ & & & \end{pmatrix}$$

$$\rho_A = \text{Tr}_B\rho = \frac{1}{2}\begin{pmatrix}\text{Tr}\begin{pmatrix} & \\ & 1\end{pmatrix} & \text{Tr}\begin{pmatrix} & -1\\ & \end{pmatrix}\\ \text{Tr}\begin{pmatrix} & \\ -1 & \end{pmatrix} & \text{Tr}\begin{pmatrix}1 & \\ & \end{pmatrix}\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}, \quad \lambda_A^1 = \frac{1}{2}, \quad \lambda_A^2 = \frac{1}{2}$$

$$S(A) = -\text{Tr}\rho_A \ln\rho_A = -\sum_i \lambda_A^i \ln\lambda_A^i = -\left(\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right) = \ln 2$$

2. 乘积态 $|\psi\rangle = \dfrac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle)$. 总密度矩阵为

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{4}\begin{pmatrix}1\\1\\1\\1\end{pmatrix}\begin{pmatrix}1 & 1 & 1 & 1\end{pmatrix} = \frac{1}{4}\begin{pmatrix}1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\end{pmatrix}$$

$$\rho_A = \text{Tr}_B\rho = \frac{1}{4}\begin{pmatrix}\text{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} & \text{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\\ \text{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} & \text{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\end{pmatrix} = \frac{1}{4}\begin{pmatrix}2 & 2\\2 & 2\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}, \quad \lambda_A^1 = 0, \quad \lambda_A^2 = 1$$

$$S(A) = -\text{Tr}\rho_A \ln\rho_A = -\sum_i \lambda_A^i \ln\lambda_A^i = -(0\ln 0 + 1\ln 1) = 0.$$

0.1.1.6　互信息

双量子比特体系, A 和 B 之间的互信息为

$$I(A:B) = S(A) + S(B) - S(A\cup B)$$

0.1.1.7　EPR 佯谬和 Bell 不等式