

Homework 1

推导公式(2.14), (2.15)

解: Schrödinger eq. $i\hbar \frac{\partial}{\partial t} \psi = H \psi$ ①

$$\text{其中 } H = \frac{1}{2\mu} (\vec{p} - \frac{q}{c} \vec{A})^2 + q\phi$$

$$\text{由①得 } -i\hbar \frac{\partial}{\partial t} \psi^* = H^* \psi^* \quad ②$$

$$\text{于是 } \psi^* i\hbar \frac{\partial}{\partial t} \psi = \psi^* H \psi$$

$$-i\hbar \frac{\partial}{\partial t} \psi^* = \psi^* H^* \psi$$

$$\text{两式相减得 } i\hbar \frac{\partial}{\partial t} (\psi^* \psi) = \psi^* H \psi - \psi H^* \psi$$

$$= \psi^* \left(\frac{1}{2\mu} (\vec{p} - \frac{q}{c} \vec{A})^2 \right) \psi - \psi \left(\frac{1}{2\mu} (\vec{p} - \frac{q}{c} \vec{A})^2 \right)^* \psi^*$$

$$= \frac{1}{2\mu} (\psi^* (-\hbar^2 \nabla^2 + \frac{q^2}{c^2} A^2 - \frac{q}{c} (2\vec{p} \cdot \vec{A})) \psi$$

$$- \psi (-\hbar^2 \nabla^2 + \frac{q^2}{c^2} A^2 - \frac{q}{c} (2\vec{p} \cdot \vec{A}))^* \psi)$$

$$= \frac{1}{2\mu} (\psi^* (-\hbar^2 \nabla^2 - \frac{q}{c} (2\vec{p} \cdot \vec{A})) \psi - \psi (-\hbar^2 \nabla^2 - \frac{q}{c} (2\vec{p} \cdot \vec{A}))^* \psi)$$

$$= \frac{1}{2\mu} (-\hbar^2 (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*) - \frac{2q}{c} (\psi^* \vec{p} \cdot \vec{A} \psi - \psi \vec{p} \cdot \vec{A}^* \psi^*))$$

$$= \frac{1}{2\mu} (-\hbar^2 \vec{\nabla} \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) + \frac{2i\hbar q}{c} (\psi^* \nabla \cdot (\vec{A} \psi) + \psi \nabla \cdot (\vec{A} \psi^*)))$$

$$= \frac{1}{2\mu} (-\hbar^2 \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) + \frac{2i\hbar q}{c} (\vec{A} \cdot \psi^* \nabla \psi + \vec{A} \cdot \psi \nabla \psi^*))$$

$$= \frac{\hbar}{2\mu} (-\hbar \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) + \frac{2i\hbar q}{c} \vec{A} \cdot \vec{\nabla} (\psi^* \psi))$$

$$\Rightarrow \frac{\partial}{\partial t} (\psi^* \psi) = \frac{1}{2\mu i} (-\hbar \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) + \frac{2i\hbar q}{c} \vec{A} \cdot \vec{\nabla} (\psi^* \psi))$$

$$= \frac{i\hbar}{2\mu} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) + \frac{q}{\mu c} \vec{A} \cdot \vec{\nabla} (\psi^* \psi)$$

$$\Rightarrow \frac{\partial}{\partial t} (\psi^* \psi) + \vec{\nabla} \cdot \left(-\frac{i\hbar}{2\mu} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q}{\mu c} \vec{A} (\psi^* \psi) \right) = 0$$

$$\text{设 } \rho = \psi^* \psi, \vec{j} = -\frac{i\hbar}{2\mu} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q}{\mu c} \vec{A} (\psi^* \psi)$$

$$= -\frac{i\hbar}{2\mu} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q}{\mu c} \vec{A} \rho$$

$$\text{则 } \frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot \vec{j} = 0$$

(2.14) 证毕

下边 \vec{j} 的定义相当于原来的几率流定义中 \vec{p} 换为机械动量：

$$\begin{aligned}
 & \frac{1}{2\mu} (\psi^* (\vec{p} - \frac{q\vec{A}}{c}) \psi + \psi (\vec{p} - \frac{q\vec{A}}{c}) \psi^*) \\
 &= \frac{1}{2\mu} (-i\hbar (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q}{c} \vec{A} (\psi^* \psi)) \\
 &= \frac{-i\hbar}{2\mu} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q}{\mu c} \vec{A} \psi \\
 &= \frac{-i\hbar}{2\mu} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q}{\mu c} \vec{A} \psi \quad \text{与之前定义的 } \vec{j} \text{ 相同. (2.15) 证毕.}
 \end{aligned}$$

Homework 2

1. 推导讲义中对易式 (2.38).

解: $\vec{\pi} = \vec{p} - q\vec{A}/c$

$$\begin{aligned}
 \text{由 } [\pi_i, \pi_j] \psi &= [p_i - \frac{qA_i}{c}, p_j - \frac{qA_j}{c}] \psi \\
 &= (p_i p_j - \frac{q}{c} p_i A_j - \frac{q}{c} A_i p_j + \frac{q^2}{c^2} A_i A_j) \psi \\
 &\quad - (p_j p_i - \frac{q}{c} p_j A_i - \frac{q}{c} A_j p_i + \frac{q^2}{c^2} A_j A_i) \psi \\
 &= (p_i p_j - p_j p_i) \psi - \frac{q}{c} (p_i A_j - A_j p_i) \psi + \frac{q}{c} (p_j A_i - A_i p_j) \psi \\
 &= -\frac{q}{c} (\psi (\nabla A_j)_i + A_j (\nabla \psi)_i - A_j (\nabla \psi)_i - \psi (\nabla A_i)_j \\
 &\quad - A_i (\nabla \psi)_j + A_i (\nabla \psi)_j) (-i\hbar) \\
 &= \frac{i\hbar q}{c} (\psi (\nabla A_j)_i - \psi (\nabla A_i)_j) \\
 &= \frac{i\hbar q}{c} ((\nabla A_j)_i - (\nabla A_i)_j) \psi
 \end{aligned}$$

$$\Rightarrow [\pi_i, \pi_j] = \frac{i\hbar q}{c} ((\nabla A_j)_i - (\nabla A_i)_j) \quad ①$$

$$\text{考虑到 } \vec{B} = \vec{\nabla} \times \vec{A} \Rightarrow B_1 = (\vec{\nabla} \times \vec{A})_1 = \frac{\partial A_3}{\partial y} - \frac{\partial A_2}{\partial z}$$

$$B_2 = (\vec{\nabla} \times \vec{A})_2 = \frac{\partial A_3}{\partial z} - \frac{\partial A_1}{\partial x}$$

$$B_3 = (\vec{\nabla} \times \vec{A})_3 = \frac{\partial A_1}{\partial y} - \frac{\partial A_2}{\partial x}$$

$$\begin{array}{ccc}
 & i & j & k \\
 \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
 A_x & A_y & A_z
 \end{array}$$

所以①表明 $[\pi_i, \pi_j] = \frac{i\hbar q}{c} \sum_{i,j,k} B_k$. 其中 $\sum_{i,j,k}$ 为三阶全反称张量. □

2. 利用该对易式. 类似角动量上升下降算符, 可定义产生消灭算符 a, a^\dagger 满足 $[a, a^\dagger] = 1$. 对比谐振子哈密顿, 写出 z 方向匀强磁场 B 中移动电子的能级公式.

$$E_{K,n} = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega(n + \frac{1}{2})$$

其中 $\omega = eB/mc$.

解: 定义 $a = \sqrt{\frac{c}{2\hbar q_B}}(\pi_x + i\pi_y) \quad a^\dagger = \sqrt{\frac{c}{2\hbar q_B}}(\pi_x - i\pi_y)$

$$\begin{aligned} \text{则 } [a, a^\dagger] &= \frac{c}{2\hbar q_B} [\pi_x + i\pi_y, \pi_x - i\pi_y] \\ &= \frac{c}{2\hbar q_B} ([\pi_x, -i\pi_y] + [i\pi_y, \pi_x]) \\ &= \frac{c}{2\hbar q_B} (-i \cdot \frac{i\hbar q}{c} B - i \cdot \frac{i\hbar q}{c} B) \end{aligned}$$

$$= \frac{c}{2\hbar q_B} \cdot \left(\frac{2\hbar q B}{c} \right) = 1 \Rightarrow aa^\dagger = a^\dagger a + 1$$

$$\pi_x = \sqrt{\frac{\hbar q B}{2c}}(a + a^\dagger) \quad \pi_y = \frac{1}{i} \sqrt{\frac{\hbar q B}{2c}}(a - a^\dagger)$$

$$H = \frac{1}{2\mu} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\varphi = \frac{1}{2\mu} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2$$

分离变量 $\psi = \psi(x, y) e^{ik_z z}$, z 方向自由运动, $E_z = \frac{\hbar^2 k_z^2}{2\mu}$

$$H_{xy} = \frac{1}{2\mu} [\pi_x^2 + \pi_y^2] = \frac{1}{2\mu} \frac{\hbar^2 B^2}{2c} [(a^2 + a^{*\dagger 2} + aa^\dagger + a^\dagger a) - (a^2 + a^{*\dagger 2} - aa^\dagger - a^\dagger a)]$$

$$= \frac{\hbar^2 B^2}{2\mu c} (aa^\dagger + a^\dagger a) = \frac{\hbar^2 B^2}{2\mu c} (2aa^\dagger + 1)$$

$$= \frac{\hbar^2 B^2}{\mu c} (a^\dagger a + \frac{1}{2}) = \hbar\omega(a^\dagger a + \frac{1}{2}) \quad \text{其中 } \omega = \frac{qB}{\mu c}$$

谐振子哈密顿 $H = (a^\dagger a + \frac{1}{2})\hbar\omega$ 能级 $E_n = (n + \frac{1}{2})\hbar\omega$

可见二者形式一致! 于是能级公式为 (对于电子, $q=e$, μ 替换为 m)

$$E_n = E_{z,n} + E_{xy,n} = \frac{\hbar^2 k_z^2}{2m} + (n + \frac{1}{2})\hbar\omega \quad \text{其中 } \omega = \frac{eB}{mc}$$

Homework 3

对称规范下，计算基态简并度。

解：基态情况下 $\eta_r=0, m=0, -1, -2, \dots$ ($\text{EP } n=0$)

故波函数中合流超几何级数项 $F(0, |m|+1, \alpha^2 r^2) = 1$

$$dp = 2\pi r^{\frac{1}{2}} \chi^2 dr = 2\pi \chi^2 dr \quad \chi = r^{|m|+\frac{1}{2}} e^{-\frac{1}{2}\alpha^2 r^2}$$

在最可几半径 $r=r_{\max}$ 处， $dp = 2\pi \chi^2 dr$ 最大

$$\text{即 } \frac{d(2\pi \chi^2)}{dr} = \frac{d}{dr}(r^{2|m|+1} e^{-\alpha^2 r^2}) = (2|m|+1)r^{2|m|} e^{-\alpha^2 r^2}$$

$$-2\alpha^2 r r^{2|m|+1} e^{-\alpha^2 r^2}$$

$$= r^{12|m|} e^{-\alpha^2 r^2} (2|m|+1 - 2\alpha^2 r^2) \text{ 在 } r=r_{\max} \text{ 时为 } 0$$

$$\Rightarrow r_{\max} = \sqrt{\frac{2|m|+1}{2\alpha^2}}$$

波函数能放在盒中的条件是 $r_{\max} < R$

$$\text{即 } 2|m|+1 < 2\alpha^2 R^2$$

$$\Rightarrow |m| < \alpha^2 R^2 - \frac{1}{2}$$

又由 m 取非正整数知

m 可能的取值为 $0, -1, -2, \dots, -[\alpha^2 R^2 - \frac{1}{2}]$

总取值个数为 $[\alpha^2 R^2 - \frac{1}{2}] + 1$ EP 为简并度

$$\text{其中方括号代表取整} \quad \alpha = \sqrt{\frac{\mu w_L}{\hbar}} = \sqrt{\frac{eB}{2\hbar c}}$$

可见基态简并度仍可写成 $\frac{BA}{hc/e}$ 的形式。

Homework 4

1. 带电粒子在互相垂直的磁场和电场中运动，求能级。

$$\vec{\Sigma} = (0, \Sigma, 0) \quad \vec{B} = (0, 0, B) \quad \phi = -\Sigma y \quad \vec{A} = (-By, 0, 0)$$

粒子的哈密顿量 $H = \frac{1}{2\mu} [(P_x + \frac{q}{c}By)^2 + P_y^2 + P_z^2] - q\Sigma y$

选取力学量完全集为 (H, P_x, P_z) ，它们的共同本征函数

$$\psi = \psi(y) \exp(i\frac{P_x}{\hbar}x) \exp(i\frac{P_z}{\hbar}z)$$

$$\begin{aligned} H &= \frac{1}{2\mu} [(P_x + \frac{q}{c}By)^2 + P_y^2 + P_z^2] - q\Sigma y \\ &= \frac{1}{2\mu} [-\hbar^2 \frac{\partial^2}{\partial x^2} + 2P_x \frac{q}{c}By + \frac{q^2 B^2}{c^2} y^2 - \hbar^2 \frac{\partial^2}{\partial y^2} - \hbar^2 \frac{\partial^2}{\partial z^2}] - q\Sigma y \\ &= \frac{1}{2\mu} (\frac{q^2 B^2}{c^2} y^2 + 2P_x \frac{q}{c}By - 2\mu q\Sigma y) - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial y^2} + \frac{1}{2\mu} (-\hbar^2 \frac{\partial^2}{\partial x^2} - \hbar^2 \frac{\partial^2}{\partial z^2}) \\ &= \frac{q^2 B^2}{2\mu c^2} (y - y_0)^2 - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial y^2} - \frac{q^2 B^2}{2\mu c^2} y_0^2 + \frac{-\hbar^2}{2\mu} (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}) \end{aligned}$$

其中 $y_0 = \frac{C^2 \mu}{q^2 B^2} (q\Sigma - \frac{P_x q}{c \mu} B)$

可见类似于一维谐振子 (y 方向)

$$\omega^2 = \frac{q^2 B^2}{\mu^2 c^2} \Rightarrow \omega = \frac{qB}{\mu c} \quad (q \text{ 为带电量的绝对值})$$

→ 能级 $E_n = (n + \frac{1}{2})\hbar\omega + \frac{P_x^2}{2\mu} + \frac{P_z^2}{2\mu} - \frac{q^2 B^2}{2\mu c^2} y_0^2, n = 0, 1, 2, \dots$

其中 ω, y_0 的定义在前面已经给出， P_x, P_z 可以取任意值。

2. 中子干涉实验：一个中子的波函数分成两束，其中一束通过宽为 l 的磁场 B ，两束飞过相等距离后汇合干涉。证明调节磁场相邻两个峰满足 $\Delta B = \frac{4\pi\hbar c}{e g_n \lambda l}$ ，其中 $g_n \cdot \frac{-e\hbar}{2m_n c}$ 是中子磁矩， λ 为中子波长。

解：中子在磁场中的势能 $V = -\vec{\mu} \cdot \vec{B} = \frac{g_n e \hbar B}{2m_n c}$

中子波长与速度的关系是 $\lambda = \frac{\hbar}{p} = \frac{2\pi\hbar}{m_n v} \Rightarrow v = \frac{2\pi\hbar}{m_n \lambda}$

所以中子在磁场中运动的时间 $t = \frac{l}{v} = \frac{l m_n \lambda}{2\pi\hbar}$

类比AB效应， $\Delta\phi = \frac{1}{\hbar} \int_0^t V dt = \frac{1}{\hbar} V t = \frac{1}{\hbar} \frac{g_n e \hbar B}{2m_n c} \frac{l m_n \lambda}{2\pi\hbar} = \frac{g_n e B l \lambda}{4\pi\hbar c}$

对于相邻的两个峰， $\Delta\phi = 2\pi$ 。于是相邻两个峰满足

$$\Delta B = \frac{4\pi\hbar c}{g_n e l \lambda} \cdot 2\pi = \frac{8\pi^2 \hbar c}{g_n e l \lambda}$$

Homework 5

考虑由自旋 $\frac{1}{2}$ 粒子构成的绝热系综，知道 $\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle$ 的符号，你能定出态来吗？为什么？

对于绝热系综，总可以把它的密度矩阵写成 $\rho = |\alpha\rangle\langle\alpha|$ ，其中 $|\alpha\rangle = \vec{n} \cdot \vec{\sigma}$ 粒子的自旋有确定的指向 \vec{n} 。而此时 $\langle \sigma_x \rangle = \sin\theta \cos\varphi, \langle \sigma_y \rangle = \sin\theta \sin\varphi, \langle \sigma_z \rangle = \cos\theta$

显然，若 $\langle \sigma_x \rangle = \langle \sigma_y \rangle = 0, \langle \sigma_z \rangle > 0$ 对应北极 A：

$\langle \sigma_x \rangle = \langle \sigma_y \rangle = 0, \langle \sigma_z \rangle < 0$ 对应南极 B。

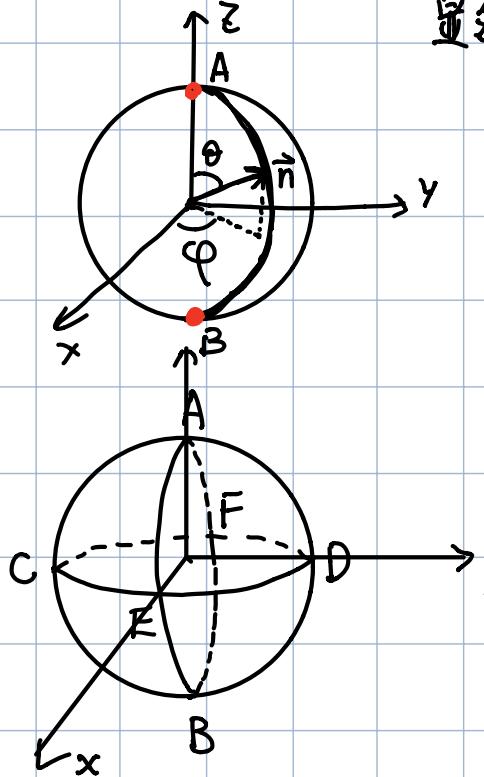
$\langle \sigma_x \rangle = \langle \sigma_z \rangle = 0, \langle \sigma_y \rangle > 0$ 对应 D

$\langle \sigma_x \rangle = \langle \sigma_z \rangle = 0, \langle \sigma_y \rangle < 0$ 对应 C

$\langle \sigma_y \rangle = \langle \sigma_z \rangle = 0, \langle \sigma_x \rangle > 0$ 对应 E

$\langle \sigma_y \rangle = \langle \sigma_z \rangle = 0, \langle \sigma_x \rangle < 0$ 对应 F

其余情况下只能确定 \vec{n} 在球面上的哪些区域而不确定具体位置（注：表中区域均不含边界）



$\langle \sigma_x \rangle$	$\langle \sigma_y \rangle$	$\langle \sigma_z \rangle$	区域	$\langle \sigma_x \rangle$	$\langle \sigma_y \rangle$	$\langle \sigma_z \rangle$	区域
+	+	+	面 AED	0	-	-	弧 CB
+	+	-	面 BED	+	0	+	弧 AE
+	-	+	面 ACE	+	0	-	弧 EB
-	+	+	面 AFD	-	0	+	弧 FA
+	-	-	面 CBE	-	0	-	弧 BF
-	+	-	面 DFB	+	+	0	弧 ED
-	-	+	面 AFC	+	-	0	弧 CE
0	+	+	弧 AD	-	-	0	弧 CF
0	+	-	弧 BD				
0	-	+	弧 AC				

Homework 6

1. 两个自旋 $\frac{1}{2}$ 粒子构成的系统哈密顿为 $H = \vec{S}_1 \cdot \vec{S}_2$. 处于温度为T的平衡状态. (取方=1)

(1) 在 (S^2, S_z) 表象写出其密度矩阵, 指出该系统由哪些能态系综按什么几率混合而成.

记以自旋 $|+\rangle$ 的态, β 为自旋 $|-\rangle$ 的态, 下角标 1, 2 分别代表 2 个自旋 $\frac{1}{2}$ 粒子.

则 (S^2, S_z) 的共同本征态与 H 的本征值为 singlet: $\frac{1}{\sqrt{2}}(\alpha_1\beta_2 - \beta_1\alpha_2) = |1\rangle$ H 本征值 $E_1 = -\frac{3}{4}$

triplet: $\frac{1}{\sqrt{2}}(\alpha_1\beta_2 + \beta_1\alpha_2) = |2\rangle$ $E_2 = \frac{1}{4}$

$\alpha_1\alpha_2 = |3\rangle$ $E_3 = \frac{1}{4}$

$\beta_1\beta_2 = |4\rangle$ $E_4 = \frac{1}{4}$

$$\text{配分函数 } Z = \sum_{i=1}^4 e^{-\beta E_i} = e^{\frac{3}{4}\beta} + 3e^{-\frac{1}{4}\beta} \text{ 其中 } \beta = \frac{1}{k_B T}$$

$$p_{11} = \frac{\exp(-\beta E_1)}{Z} = \frac{1}{1+3e^{-\beta}} \quad p_{22} = p_{33} = p_{44} = \frac{\exp(-\frac{1}{4}\beta)}{Z} = \frac{e^{-\beta}}{1+3e^{-\beta}}$$

密度矩阵 $\rho = \frac{1}{1+3e^{-\beta}} \begin{pmatrix} 1 & e^{-\beta} & e^{-\beta} & e^{-\beta} \\ e^{-\beta} & 1 & e^{-\beta} & e^{-\beta} \\ e^{-\beta} & e^{-\beta} & 1 & e^{-\beta} \\ e^{-\beta} & e^{-\beta} & e^{-\beta} & 1 \end{pmatrix}$ 该系统由 $|1\rangle, |2\rangle, |3\rangle, |4\rangle$ 四种能态以各自几率分别为 $\frac{1}{1+3e^{-\beta}}, \frac{e^{-\beta}}{1+3e^{-\beta}}, \frac{e^{-\beta}}{1+3e^{-\beta}}, \frac{e^{-\beta}}{1+3e^{-\beta}}$ 混合而成

(2) 在 (S^2, S_x) 表象写出其密度矩阵, 指出该系统由哪些能态混合而成? 将该密度矩阵变换到

(S^2, S_z) 表象

记 $|+\rangle$ 为自旋 $|+\rangle_x$ 的态, $|-\rangle$ 为自旋 $|-\rangle_x$ 的态. 则 (S^2, S_x) 的共同本征态与本征值为

$$\frac{1}{\sqrt{2}}(|+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2) = |1^0\rangle, E_1 = -\frac{3}{4}. \quad \frac{1}{\sqrt{2}}(|+\rangle_1|+\rangle_2 + |-\rangle_1|-\rangle_2) = |2^0\rangle, E_2 = \frac{1}{4}$$

$$|+\rangle_1|+\rangle_2 = |3^0\rangle, E_3 = \frac{1}{4} \quad |-\rangle_1|-\rangle_2 = |4^0\rangle, E_4 = \frac{1}{4}$$

类似(1)的过程, 密度矩阵数值同上(但选取的基矢已经不同)

该系统由 $|1^0\rangle, |2^0\rangle, |3^0\rangle, |4^0\rangle$ 四种能态以各自几率分别为 $\frac{1}{1+3e^{-\beta}}, \frac{e^{-\beta}}{1+3e^{-\beta}}, \frac{e^{-\beta}}{1+3e^{-\beta}}, \frac{e^{-\beta}}{1+3e^{-\beta}}$ 混合而成

$$|1^0\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{2}(\alpha_1 + \beta_1)(\alpha_2 - \beta_2) - \frac{1}{2}(\alpha_1 - \beta_1)(\alpha_2 + \beta_2)\right) = \frac{1}{\sqrt{2}}(-\alpha_1\beta_2 + \beta_1\alpha_2) = -|1\rangle$$

$$|2^0\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{2}(\alpha_1 + \beta_1)(\alpha_2 - \beta_2) + \frac{1}{2}(\alpha_1 - \beta_1)(\alpha_2 + \beta_2)\right) = \frac{1}{\sqrt{2}}(\alpha_1\alpha_2 - \beta_1\beta_2) = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle)$$

$$|3^0\rangle = (\alpha_1 + \beta_1)(\alpha_2 + \beta_2) \cdot \frac{1}{2} = \frac{1}{2}(\alpha_1\alpha_2 + \beta_1\beta_2 + \alpha_1\beta_2 + \beta_1\alpha_2) = \frac{1}{2}(|3\rangle + |4\rangle) + \sqrt{2}|2\rangle$$

$$|4^0\rangle = (\alpha_1 - \beta_1)(\alpha_2 - \beta_2) \cdot \frac{1}{2} = \frac{1}{2}(\alpha_1\alpha_2 + \beta_1\beta_2 - (\alpha_1\beta_2 + \beta_1\alpha_2)) = \frac{1}{2}(|3\rangle + |4\rangle) - \sqrt{2}|1\rangle$$

$$\therefore U = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{\sqrt{2}}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad \therefore \text{变换到 } (S_x, S_y, S_z) \text{ 表象为 } U^{-1} \rho U = \frac{1}{1+3e^{-\beta}} \begin{pmatrix} 1 & e^{-\beta} & e^{-\beta} \\ e^{-\beta} & e^{-\beta} & e^{-\beta} \\ e^{-\beta} & e^{-\beta} & e^{-\beta} \end{pmatrix}$$

与(i) 得到的结果相同.

(3) 求出 S_1 的纯化密度矩阵. 计算 $\langle (S_x(1), S_y(1), S_z(1)) \rangle$.

$$\begin{aligned} P_1 = \text{tr}_2 \rho &= \frac{1}{1+3e^{-\beta}} [(\langle \alpha_2 | ① \rangle \langle ① | \alpha_2 \rangle + \langle \beta_2 | ① \rangle \langle ① | \beta_2 \rangle) + e^{-\beta} (\langle \alpha_2 | ② \rangle \langle ② | \alpha_2 \rangle + \langle \beta_2 | ② \rangle \langle ② | \beta_2 \rangle) \\ &\quad + \langle \alpha_2 | ③ \rangle \langle ③ | \alpha_2 \rangle + \langle \beta_2 | ③ \rangle \langle ③ | \beta_2 \rangle + \langle \alpha_2 | ④ \rangle \langle ④ | \alpha_2 \rangle + \langle \beta_2 | ④ \rangle \langle ④ | \beta_2 \rangle] \\ &= \frac{1}{1+3e^{-\beta}} [(\frac{1}{2} |\beta_1\rangle \langle \beta_1| + \frac{1}{2} |\alpha_1\rangle \langle \alpha_1|) + e^{-\beta} (\frac{1}{2} |\beta_1\rangle \langle \beta_1| + \frac{1}{2} |\alpha_1\rangle \langle \alpha_1| + |\alpha_1\rangle \langle \alpha_1| + |\beta_1\rangle \langle \beta_1|)] \end{aligned}$$

纯化密度矩阵: $P_1 = \frac{1}{1+3e^{-\beta}} \begin{pmatrix} \frac{1}{2} + \frac{3}{2}e^{-\beta} & 0 \\ 0 & \frac{1}{2} + \frac{3}{2}e^{-\beta} \end{pmatrix} = \frac{1}{2} I$

$$\langle S_x(1) \rangle = \frac{1}{2} \text{tr}(P_1 \sigma_x) = \frac{1}{2} \cdot \frac{1}{2} \text{tr}(I \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}) = 0$$

同理:

$$\langle S_y(1) \rangle = \frac{1}{2} \text{tr}(P_1 \sigma_y) = 0 \quad \langle S_z(1) \rangle = \frac{1}{2} \text{tr}(P_1 \sigma_z) = 0$$

$$\therefore \langle (S_x(1), S_y(1), S_z(1)) \rangle = (\langle S_x(1) \rangle, \langle S_y(1) \rangle, \langle S_z(1) \rangle) = (0, 0, 0)$$

2. 计算纠缠熵证明 $| \alpha \rangle = \frac{1}{2} (| 0 \rangle_A | 1 \rangle_B + | 1 \rangle_A | 0 \rangle_B + | 0 \rangle_A | 0 \rangle_B + | 1 \rangle_A | 0 \rangle_B)$ 不是纠缠态。

解: $P_{AB} = | \alpha \rangle \langle \alpha |$

选 H_B 的基矢为 $| 0 \rangle_B$ 和 $| 1 \rangle_B$, 则 纯化密度算符

$$\begin{aligned} P_A = \text{tr}_B P_{AB} &= \langle 0 | \alpha \rangle \langle \alpha | 0 \rangle_B + \langle 1 | \alpha \rangle \langle \alpha | 1 \rangle_B \\ &= \frac{1}{4} [(| 0 \rangle_A + | 1 \rangle_A)(A \langle 0 | + A \langle 1 |) + (| 0 \rangle_A + | 1 \rangle_A)(A \langle 0 | + A \langle 1 |)] \\ &= \frac{1}{2} (| 0 \rangle_A \langle 0 | + | 0 \rangle_A \langle 1 | + | 1 \rangle_A \langle 0 | + | 1 \rangle_A \langle 1 |) \end{aligned}$$

选 H_A 的基矢为 $| 0 \rangle_A$ 和 $| 1 \rangle_A$, 则 纯化密度矩阵

$$P_A = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \xrightarrow{\text{对角化}} P_A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \Rightarrow S = -\text{tr} P_A \log P_A = -1 \cdot \log 1 = 0$$

纠缠熵为 0, 故 $| \alpha \rangle$ 不是纠缠态。