0.1 单项选择

1. **让大量热化的自旋通过 Stern-Gerlach 装置SG $\hat{z}$,测得 S_+^z 的概率是?**

   大量热化自旋表示充分随机, 所以 $P(S_+^z) = ||\chi_+^{z\dagger}\frac{1}{\sqrt{2}}(\chi_+^z + \chi_-^z)||^2 = \boxed{\frac{1}{2}}$

2. **Pauli 矩阵 $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, 那么 $\sigma^x\sigma^z$ 等于?**

   $\sigma^x\sigma^z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

3. **混态可以用混态的密度矩阵来描述. 假设系统处于态 $|\phi_i\rangle$ 的概率为 p_i, 注意 $\sum_i p_i = 1$, 那么该系统的密度矩阵为 $\rho = \sum_i |\phi_i\rangle p_i \langle\phi_i|$, 那么 Tr$[\rho]$ 应满足?**

   因为密度矩阵的迹表示系统的总概率, 而概率必须归一化, 即 $\mathrm{Tr}[\rho] = \sum_i p_i = \boxed{1}$

4. **如果 ρ 是混态的密度矩阵, 那么 Tr$[\rho^2]$ 应满足?**

   对任意密度矩阵总有$\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$. 那么$\hat{\rho}^2 = \sum_\alpha p_\alpha|\psi_\alpha\rangle\langle\psi_\alpha| \sum_\beta p_\beta |\psi_\beta\rangle\langle\psi_\beta| = \sum_\alpha p_\alpha^2 |\psi_\alpha\rangle\langle\psi_\alpha|$. 对于纯态($p_n^2 = p_n$) $\mathrm{Tr}[\rho^2] = \mathrm{Tr}[\rho] = 1$, 而混态($p_n^2 \neq p_n$)则是 $\mathrm{Tr}[\rho^2]\boxed{<1}$.

5. **考虑系统哈密顿量 H 不显含时间, 时间演化算符为 $U(t,0) = e^{-iHt/\hbar}$. 在海森堡绘景中, 我们让算符承载时间演化, 海森堡绘景中的算符定义为 $A_H(t) = U^\dagger(t,0)AU(t,0)$, 其中 A 是薛定谔绘景中的算符, 如果 A 不显含时间, 那么 $\mathrm{d}A_H(t)/\mathrm{d}t$ 等于?**

$$
\begin{aligned}
\frac{\mathrm{d}A_H(t)}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}Ae^{-iHt/\hbar}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}\right)Ae^{-iHt/\hbar} + e^{iHt/\hbar}\frac{\mathrm{d}}{\mathrm{d}t}\left(Ae^{-iHt/\hbar}\right) \\
&= \frac{iH}{\hbar}e^{iHt/\hbar}Ae^{-iHt/\hbar} - e^{iHt/\hbar}A\frac{iH}{\hbar}e^{-iHt/\hbar} = \frac{i}{\hbar}\left(He^{iHt/\hbar}Ae^{-iHt/\hbar} - e^{iHt/\hbar}Ae^{-iHt/\hbar}H\right) \\
&= \frac{i}{\hbar}[H, A_H(t)] = \boxed{\frac{1}{i\hbar}[A_H(t), H]}
\end{aligned}
$$

6. **电磁场中电荷为 q 的单粒子哈密顿量为 $H = \frac{(\vec{p} - q\vec{A})^2}{2m} + q\phi$, 那么薛定谔方程 $i\hbar\frac{\partial\psi}{\partial t} = H\psi$ 满足规范不变性: $\vec{A} \to \vec{A} - \nabla\Lambda$, $\phi \to \phi + \frac{\partial\Lambda}{\partial t}$, $\psi \to$?**

   推导极其麻烦, 建议直接背结论, 不要试图考场现推. 假设 $\psi' = \psi e^{if(\vec{r},t)}$ 是满足规范变换的, 其中 $f(\vec{r},t)$ 是待定函数. 连同其它的规范变换, 代入薛定谔方程得到 $f(\vec{r},t)$ 的微分方程:

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\left[\psi e^{if(\vec{r},t)}\right] &= \left[\frac{(-i\hbar\vec{\nabla} - q(\vec{A} - \vec{\nabla}\Lambda))^2}{2m} + q\left(\phi + \frac{\partial\Lambda}{\partial t}\right)\right]\left[\psi e^{if(\vec{r},t)}\right] \\
i\hbar\frac{\partial}{\partial t}\left[\psi e^{if(\vec{r},t)}\right] &= \left[i\hbar\frac{\partial\psi}{\partial t} - \hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)} \\
\vec{\nabla}\left(\psi e^{if(\vec{r},t)}\right) &= \left(\vec{\nabla}\psi + \psi i\vec{\nabla}f\right)e^{if(\vec{r},t)} \\
\left[-i\hbar\vec{\nabla} - q(\vec{A} - \vec{\nabla}\Lambda)\right]\left[\psi e^{if(\vec{r},t)}\right] &= \left[-i\hbar\vec{\nabla}\psi + \hbar\psi\vec{\nabla}f - q(\vec{A} - \vec{\nabla}\Lambda)\psi\right]e^{if(\vec{r},t)}
\end{aligned}
$$

$$
\begin{aligned}
&\left[-i\hbar\vec{\nabla}-q(\vec{A}-\vec{\nabla}\Lambda)\right]^2[\psi e^{if(\vec{r},t)}]=\left[-i\hbar\vec{\nabla}-q(\vec{A}-\vec{\nabla}\Lambda)\right]\left\{\left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]e^{if(\vec{r},t)}\right\}\\
&=(-i\hbar)\left\{\left[-i\hbar\nabla^2\psi+\hbar(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)+\hbar\psi\nabla^2 f-q(\vec{\nabla}\cdot\vec{A}-\nabla^2\Lambda)\psi-q(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\right]e^{if(\vec{r},t)}\right.\\
&\left.+\left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]\cdot i(\vec{\nabla}f)e^{if(\vec{r},t)}\right\}\\
&-q(\vec{A}-\vec{\nabla}\Lambda)\cdot\left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]e^{if(\vec{r},t)}
\end{aligned}
$$

展开变换前的薛定谔方程:

$$
i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{(-i\hbar\vec{\nabla}-q\vec{A})^2}{2m}+q\phi\right]\psi=-\frac{\hbar^2}{2m}\nabla^2\psi+\frac{i\hbar q}{2m}(\vec{\nabla}\cdot\vec{A})\psi+\frac{i\hbar q}{m}\vec{A}\cdot(\vec{\nabla}\psi)+\frac{q^2A^2}{2m}\psi+q\phi\psi \tag{①}
$$

展开变换后的薛定谔方程:

$$
\begin{aligned}
&\left[i\hbar\frac{\partial\psi}{\partial t}-\hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)}\\
&=e^{if(\vec{r},t)}\left[-\frac{\hbar^2}{2m}\nabla^2\psi-\frac{i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)-\frac{i\hbar^2}{2m}\psi\nabla^2 f+\frac{i\hbar q}{2m}(\vec{\nabla}\cdot\vec{A}-\nabla^2\Lambda)\psi+\frac{i\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\right.\\
&+\frac{-i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)+\frac{\hbar^2}{2m}(\vec{\nabla}f)^2\psi-\frac{\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi\\
&+\frac{i\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)(\vec{\nabla}\psi)-\frac{q\hbar}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi+\frac{q^2}{2m}(\vec{A}-\vec{\nabla}\Lambda)^2\psi\\
&\left.+q\left(\phi+\frac{\partial\Lambda}{\partial t}\right)\psi\right]
\end{aligned}\tag{②}
$$

(②) − (①) $\cdot e^{if(\vec{r},t)}$, 得到

$$
\begin{aligned}
&\left[\cancel{i\hbar\frac{\partial\psi}{\partial t}}-\hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)}\\
&=e^{if(\vec{r},t)}\left[\cancel{-\frac{\hbar^2}{2m}\nabla^2\psi}-\frac{i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)-\frac{i\hbar^2}{2m}\psi\nabla^2 f+\frac{i\hbar q}{2m}(\cancel{\vec{\nabla}\cdot\vec{A}}-\nabla^2\Lambda)\psi+\frac{i\hbar q}{2m}(\cancel{\vec{A}}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\right.\\
&+\frac{-i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)+\frac{\hbar^2}{2m}(\vec{\nabla}f)^2\psi-\frac{\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi\\
&+\frac{i\hbar q}{2m}(\cancel{\vec{A}}-\vec{\nabla}\Lambda)(\vec{\nabla}\psi)-\frac{q\hbar}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi+\frac{q^2}{2m}\left(\cancel{A^2}+(\vec{\nabla}\Lambda)^2-2\vec{A}\cdot(\vec{\nabla}\Lambda)\right)\psi\\
&\left.+q\left(\cancel{\phi}+\frac{\partial\Lambda}{\partial t}\right)\psi\right]
\end{aligned}
$$

$$
\begin{aligned}
-\hbar\psi\frac{\partial f}{\partial t}=&-\frac{i\hbar^2}{m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)-\frac{i\hbar^2}{2m}\psi\nabla^2 f-\frac{i\hbar q}{2m}\psi\nabla^2\Lambda-\frac{i\hbar q}{m}(\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\\
&+\frac{\hbar^2}{2m}\psi(\nabla f)^2-\frac{\hbar q}{m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi\\
&+\frac{q^2}{2m}\left[(\vec{\nabla}\Lambda)^2-2\vec{A}\cdot(\vec{\nabla}\Lambda)\right]\psi\\
&+q\frac{\partial\Lambda}{\partial t}\psi
\end{aligned}
$$

重点观察含 $\vec{A}$ 的项, 由于需要对任意 $\vec{A}$ 都成立, 所以 $\vec{A}$ 的系数必须为 0, 即

$$
\vec{A}\cdot\left(-\frac{\hbar q}{m}\vec{\nabla}f-\frac{q^2}{2m}2\vec{\nabla}\Lambda\right)=0
$$

最简单的解法即 $f = \dfrac{-q\Lambda}{\hbar}$, 所以规范变换后的波函数为 $\psi' = \boxed{\psi e^{-iq\Lambda/\hbar}}$. 需要关注一开始给出的 Λ 的符号, 从而影响整体变换的正负.

$$\begin{cases} \vec{A} \to \vec{A} - \nabla\Lambda \\ \phi \to \phi + \dfrac{\partial\Lambda}{\partial t} \\ \psi \to \psi \exp\left(-\dfrac{iq\Lambda}{\hbar}\right) \end{cases}, \quad \begin{cases} \vec{A} \to \vec{A} + \nabla\Lambda \\ \phi \to \phi - \dfrac{\partial\Lambda}{\partial t} \\ \psi \to \psi \exp\left(+\dfrac{iq\Lambda}{\hbar}\right) \end{cases}$$

7. **角动量的对易关系为 $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$, 升降算符定义为 $J_\pm = J_x \pm iJ_y$, 那么 $[J_+, J_-] =$?**

$$\begin{aligned} [J_+, J_-] &= [J_x + iJ_y, J_x - iJ_y] \\ &= [J_x, J_x] - i[J_x, J_y] + i[J_y, J_x] + [J_y, J_y] = -2i[J_x, J_y] = -2i(i\hbar J_z) \\ &= \boxed{2\hbar J_z} \end{aligned}$$

8. **二维谐振子的哈密顿量为 $H = \hbar\omega\left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1\right)$ 其第一激发态的简并度为?**

二维谐振子的哈密顿量用粒子数算符写作 $\hat{H} = \hbar\omega\left(\hat{n}_1 + \hat{n}_2 + \dfrac{1}{2}\right)$, 所以第一激发态即 $n_1 + n_2 = 1$, 这代表了 $|01\rangle$ 和 $|10\rangle$ 两个正交态, 所以简并度为 $\boxed{2}$.

9. **量子比特 A 和 B 构成双量子比特体系, 双量子比特态 $|\psi\rangle$ 中量子比特 A 的纠缠熵定义为 $S(A) = -\mathbf{Tr}[\rho_A \ln \rho_A]$, 其中 ρ_A 是约化密度矩阵, 由密度矩阵求迹掉量子比特 B 的自由度得到. 考虑自旋单态 $|\psi\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, 计算可得量子比特 A 的纠缠熵为?**

密度矩阵为

$$\begin{aligned} \rho = |\psi\rangle\langle\psi| &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_A \otimes |\downarrow\rangle_B - |\downarrow\rangle_A \otimes |\uparrow\rangle_B)\frac{1}{\sqrt{2}}(\langle\uparrow|_A\langle\downarrow|_B - \langle\downarrow|_A\langle\uparrow|_B) \\ &= \frac{1}{2}(|\uparrow\rangle_A\langle\uparrow|_A \otimes |\downarrow\rangle_B\langle\downarrow|_B - |\uparrow\rangle_A\langle\downarrow|_A \otimes |\downarrow\rangle_B\langle\uparrow|_B - |\downarrow\rangle_A\langle\uparrow|_A \otimes |\uparrow\rangle_B\langle\downarrow|_B + |\downarrow\rangle_A\langle\downarrow|_A \otimes |\uparrow\rangle_B\langle\uparrow|_B) \end{aligned}$$

接下来进行部分求迹, 从而得到所需的约化密度矩阵 ρ_A. 迹被定义为对角线元素之和, 所以我们通过矢量 $\mathbb{I}_A \otimes |\uparrow\rangle_B$ 和$\mathbb{I}_A \otimes |\downarrow\rangle_B$ 来提取对角元素. 具体方法是

$$\begin{aligned} (\mathbb{I}_A \otimes \langle\uparrow|_B)\rho(\mathbb{I}_A \otimes |\uparrow\rangle_B) &= \frac{1}{2}|\downarrow\rangle_A\langle\downarrow|_A, \\ (\mathbb{I}_A \otimes \langle\downarrow|_B)\rho(\mathbb{I}_A \otimes |\downarrow\rangle_B) &= \frac{1}{2}|\uparrow\rangle_A\langle\uparrow|_A, \\ \Rightarrow \rho_A = \sum_i^{\uparrow,\downarrow}(\mathbb{I}_A \otimes \langle i|_B)\rho(\mathbb{I}_A \otimes |i\rangle_B) &= \frac{1}{2}(|\downarrow\rangle_A\langle\downarrow|_A + |\uparrow\rangle_A\langle\uparrow|_A) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

由于 ρ_A 已经是对角阵, 所以对角线上元素即为特征值 $\lambda_{A,i}$. 计算 ρ_A 的纠缠熵:

$$\begin{aligned} S(A) &= -\mathrm{Tr}[\rho_A \ln \rho_A] = -\sum_i^{\uparrow,\downarrow} \lambda_{A,i} \ln \lambda_{A,i} \\ &= -\left(\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right) = \boxed{\ln 2 = 1\ \mathrm{bit}} \end{aligned}$$

10. **假设哈密顿量 H 是厄密的, 其基态能量为 E_0, 给定某个态Ψ, 测得能量期望值为 $E[\Psi]=\dfrac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$, $E(\Psi)$ 和 E_0 的关系为?**

任意态均可通过基矢展开, 形式为 $|\Psi\rangle=\sum\limits_n|n\rangle\langle n|\Psi\rangle$, 则

$$\begin{aligned}
E[\Psi]&=\left(\sum_m\langle\Psi|m\rangle\langle m|\right)\hat{H}\left(\sum_n|n\rangle\langle n|\Psi\rangle\right)=\sum_{m,n}\langle\Psi|m\rangle\langle m|\hat{H}|n\rangle\langle n|\Psi\rangle\\
&=\sum_{m,n}c_m^*E_n\delta_{mn}c_n=\sum_n|c_n|^2E_n\geq\sum_n|c_n|^2E_0=E_0
\end{aligned}$$