证明 $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ 反对易:

$[\hat{\sigma}_y, \hat{\sigma}_z] = \hat{\sigma}_y\hat{\sigma}_z - \hat{\sigma}_z\hat{\sigma}_y = 2i\hat{\sigma}_x$.

左乘 $\hat{\sigma}_y$ 有 $\hat{\sigma}_y^2\hat{\sigma}_z - \hat{\sigma}_y\hat{\sigma}_z\hat{\sigma}_y = 2i\hat{\sigma}_y\hat{\sigma}_x$, 右乘 $\hat{\sigma}_y$ 有 $\hat{\sigma}_y\hat{\sigma}_z\hat{\sigma}_y - \hat{\sigma}_z\hat{\sigma}_y^2 = 2i\hat{\sigma}_x\hat{\sigma}_y$.

两式相加. $\hat{\sigma}_y^2\hat{\sigma}_z - \hat{\sigma}_z\hat{\sigma}_y^2 = 2i(\hat{\sigma}_y\hat{\sigma}_x + \hat{\sigma}_x\hat{\sigma}_y)$, $\hat{\sigma}_y^2 = I$ ∴ $\hat{\sigma}_y\hat{\sigma}_x + \hat{\sigma}_x\hat{\sigma}_y = 0$

同理得到其它

∵ $\hat{\sigma}_z\hat{\sigma}_x = -\hat{\sigma}_x\hat{\sigma}_z$, $\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. 设 $\hat{\sigma}_x = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$

∴ 由上式得 $a = d = 0$, $\hat{\sigma}_x = \begin{pmatrix} 0 & b \\ c & 0 \end{pmatrix}$

又∵ $\hat{\sigma}_x$ 是厄密算符. $\hat{\sigma}_x^\dagger = \hat{\sigma}_x \Rightarrow \begin{pmatrix} 0 & c^* \\ b^* & 0 \end{pmatrix} = \begin{pmatrix} 0 & b \\ c & 0 \end{pmatrix}$ ($\hat{\sigma}_x^{*T} = \hat{\sigma}_x$).

又∵ $\hat{\sigma}_x^2 = I$ ∴ $b = e^{i\theta}$, $c = e^{-i\theta}$. 取 $\theta = 0$, $\hat{\sigma}_x = \cancel{\frac{\hbar}{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

同理 $\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

∴ $\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $S_x = \frac{1}{2}\hbar$ 时, $\psi = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$; $S_x = -\frac{1}{2}\hbar$ 时. $\psi = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $S_y = \frac{1}{2}\hbar$ 时. $\psi = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ i \end{pmatrix}$; $S_y = -\frac{1}{2}\hbar$ 时. $\psi = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

例: $S_z = \frac{\hbar}{2}$, 测 S_x 的值和 P

解: $S_z = \frac{\hbar}{2} \Rightarrow \phi = (1, 0)^T \triangleq a_{2\times1}$

$S_x = \frac{\hbar}{2}$ 时. $\psi = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})^T \triangleq b_{2\times1}$ ∴ $P = |b_{2\times1}^{T*} a_{2\times1}|^2 = \frac{1}{2}$

$S_x = -\frac{\hbar}{2}$ 时. $\psi = (\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2})^T \triangleq c_{2\times1}$ ∴ $P = |c_{2\times1}^{T*} a_{2\times1}|^2 = \frac{1}{2}$

例: 速度为 v, 自旋 $S = \frac{\hbar}{2}$ 的中性粒子, 沿 X 方向通过长 L 的 x 方向 B. 自旋磁矩 $\vec{M} = g\vec{S}$

问通过磁场后后, $S_z = \frac{\hbar}{2}$ 与 $S_z = -\frac{\hbar}{2}$ 的粒子的比例 2) 若全是 $S_z = -\frac{\hbar}{2}$ 的粒子, 求 B

解: $\hat{H} = -\vec{M}\cdot\vec{B} = -g\hat{S}\cdot\vec{B}_x = -gB\hat{S}_x$, $\hat{H}\phi = E\phi \Rightarrow -gB\hat{S}_x\phi = E\phi$

$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ∴ $E = \pm\frac{\hbar}{2}gB$. $E_1 = -\frac{gB\hbar}{2} \triangleq \omega_1\hbar$, $E_2 = \frac{gB\hbar}{2} \triangleq \omega_2\hbar$

在 $\psi(\vec{r}, t)$ 中时间项为 $e^{-\frac{i}{\hbar}Et}$ ∴ 记 $\psi(t) = c_1 e^{-i\omega_1 t}\psi_1 + c_2 e^{-i\omega_2 t}\psi_2$

$c_1 = |(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})^* \cdot (1, 0)^T| = \frac{\sqrt{2}}{2}$, $c_2 = |(\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}) \cdot (1, 0)^T| = -\frac{\sqrt{2}}{2}$ (用 $\phi(0)$ 也能解)

$\psi_1 = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})^T$, $\psi_2 = (\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2})^T \Rightarrow \psi(t) = \frac{1}{\sqrt{2}}(e^{-i\omega_1 t}\psi_1 + e^{-i\omega_2 t}\psi_2) = \begin{pmatrix} \cos\omega t \\ -i\sin\omega t \end{pmatrix}$

∴ $\psi(\frac{L}{v}) = (\ \cdot\ )$ $P = |c_1(\frac{L}{v})|^2 / |c_2(\frac{L}{v})|^2$

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例：将一个自旋 $s=\frac{1}{2}$ 的粒子放在 $\vec{B}=B_0(\sin\omega t\,\vec{i}+\cos\omega t\,\vec{k})$ 内，已知自旋磁矩 $\vec{M}=2M\hat{S}$，求 $\hat{H}$ 的本征值和本征矢

解：$\hat{H}=-\vec{M}\cdot\vec{B}=-2M\hat{S}\cdot\vec{B}=-2MB_0(\hat{S}_x\sin\omega t+\hat{S}_z\cos\omega t)$

$\hat{S}_x=\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$，$\hat{S}_z=\frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$\therefore\ \hat{H}=-\hbar MB_0\begin{pmatrix}\cos\omega t&\sin\omega t\\\sin\omega t&-\cos\omega t\end{pmatrix}$

$\therefore\ \hat{H}\psi=E\psi\ \Rightarrow\ E=\pm\hbar MB_0$

$E=-\hbar MB_0$ 时，$\phi=(\cos\frac{\omega t}{2},\sin\frac{\omega t}{2})^T$

$E=\hbar MB_0$ 时，$\phi=(\sin\frac{\omega t}{2},-\cos\frac{\omega t}{2})^T$

例：$\vec{n}=(x,y,z)$，在 σ 的表象中，求 $\sigma_n=\vec{\sigma}\cdot\vec{n}$ 的本征值和本征矢。

解：$\vec{n}=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$，$\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$

$\therefore\ \hat{\sigma}_n=\sin\theta\cos\varphi\,\hat{\sigma}_x+\sin\theta\sin\varphi\,\hat{\sigma}_y+\cos\theta\,\hat{\sigma}_z=\begin{pmatrix}\cos\theta&\sin\theta e^{-i\varphi}\\\sin\theta e^{i\varphi}&-\cos\theta\end{pmatrix}$

$\therefore\ \hat{\sigma}_n\psi=\lambda\psi$，$\hat{S}_n=\frac{\hbar}{2}\hat{\sigma}_n$

$\Rightarrow\ \lambda=\pm1$

当 $\lambda=1$ 时，$\psi=(\cos\frac{\theta}{2},\sin\frac{\theta}{2}e^{i\varphi})^T$；当 $\lambda=-1$ 时，$\psi=(-\sin\frac{\theta}{2}e^{-\frac{i\varphi}{2}},\cos\frac{\theta}{2}e^{\frac{i\varphi}{2}})^T$

例：$S_z=\frac{\hbar}{2}$，~~确定~~若自旋方向与z轴成θ角，求 $S=$，$P=$；$\bar{S}=$

解：$\hat{S}=\hat{S}_x\vec{i}+\hat{S}_y\vec{j}+\hat{S}_z\vec{k}=\hat{S}_n=\frac{\hbar}{2}\hat{\sigma}_n$，$\hat{\sigma}_n$ 见上例.

$S_z=\frac{\hbar}{2}\Rightarrow\psi_1=(1,0)^T$

当 $S=\frac{\hbar}{2}$ 时，$\psi_2=(\cos\frac{\theta}{2},\sin\frac{\theta}{2}e^{i\varphi})^T\Rightarrow P=|\psi_2^{T*}\cdot\psi_1|^2=\cos^2\frac{\theta}{2}$

当 $S=-\frac{\hbar}{2}$ 时，$\psi_3=(-\sin\frac{\theta}{2}e^{-\frac{i\varphi}{2}},\cos\frac{\theta}{2}e^{\frac{i\varphi}{2}})^T\Rightarrow P=|\psi_3^{\dagger}\cdot\psi_1|^2=\sin^2\frac{\theta}{2}$

$\bar{S}=\sum S_i^2 P_i=\frac{\hbar}{2}(\cos^2\frac{\theta}{2}-\sin^2\frac{\theta}{2})=\frac{\hbar}{2}\cos\theta$

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例：自旋投影算符 $\hat{S}_n=\frac{\hbar}{2}\vec{\sigma}\cdot\vec{n}$，$S_z=\frac{\hbar}{2}$，在 $\hat{\sigma}_n=\vec{\sigma}\cdot\vec{n}$ 的本征值为1的态中，

求 $\sigma_y=?$，$P=?$

解：由前例，$\sigma_n=1$ 时，$\psi=(\cos\frac{\theta}{2},\sin\frac{\theta}{2}e^{i\varphi})^T$

$\sigma_y=1$ 时，$\psi_2=(\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}i)^T$，$P=|\psi_2^\dagger\cdot\psi|^2=(1+\sin\theta\sin\varphi)\frac{1}{2}$

$\sigma_y=-1$ 时 $\psi_3=(\frac{\sqrt{2}}{2},-\frac{\sqrt{2}}{2}i)^T$ $P=(1-\sin\theta\sin\varphi)\frac{1}{2}$

~~核~~磁共振（电子）

在磁场中，$\hat{H}=-\vec{M}\cdot\vec{B}=\frac{q}{m}\vec{S}\cdot\vec{B}$ $\vec{S}=\vec{S}_x+\vec{S}_y+\vec{S}_z$

若 $\vec{B}=B_0\cos\omega t\,\vec{i}+B_0\sin\omega t\,\vec{j}+B\vec{k}$，则 $\hat{H}=\frac{q}{mc}(\hat{S}_xB_x+\hat{S}_yB_y+\hat{S}_zB_z)$

$\Rightarrow \hat{H}=\frac{q}{m}\frac{\hbar}{2}\begin{pmatrix}B & B_0e^{-i\omega t}\\ B_0e^{i\omega t} & -B\end{pmatrix}$

不考虑粒子空间运动，在 $t=0$ 时 $\psi(S_z,t)=\psi(\frac{\hbar}{2},0)=\begin{pmatrix}1\\0\end{pmatrix}$.

记 $\psi(S_z,t)=(a(t),b(t))^T$，求 $\forall t$，$P(S_z=-\frac{\hbar}{2})=?$

~~由薛~~ 由薛定谔方程 $E\psi=\hat{H}\psi\Rightarrow i\hbar\frac{\partial}{\partial t}\psi(S_z,t)=\frac{q}{m}\frac{\hbar}{2}\begin{pmatrix}B & B_0e^{-i\omega t}\\ B_0e^{i\omega t} & -B\end{pmatrix}\psi(S_z,t)$

$\Rightarrow\begin{cases} i\hbar\frac{\partial}{\partial t}a=\frac{\hbar e}{2m}Ba+\frac{\hbar e}{2m}B_0e^{-i\omega t}b \\ i\hbar\frac{\partial}{\partial t}b=\frac{\hbar e}{2m}B_0e^{i\omega t}a-\frac{\hbar e}{2m}Bb\end{cases}$ 令 $\frac{\hbar e}{m}B=\Omega$，$\frac{\hbar e}{m}B_0=\Omega_0$

$\Rightarrow\begin{cases} i\hbar\frac{\partial}{\partial t}a=\frac{\Omega}{2}a+\frac{\Omega_0}{2}e^{-i\omega t}b \\ i\hbar\frac{\partial}{\partial t}b=\frac{\Omega_0}{2}e^{i\omega t}a-\frac{\Omega}{2}b\end{cases}\Rightarrow\frac{d^2}{dt^2}\cdots$

$P(S_z=-\frac{\hbar}{2})=|b(t)|^2=\frac{(\Omega_0)^2}{(\omega-\Omega)^2+\Omega_0^2}\sin^2[\frac{\sqrt{(\omega-\Omega)^2+\Omega_0^2}}{2}t]$.

def $\omega=\Omega=\frac{qB}{M}$ 为拉比振荡频率.

当 $\omega=\Omega$ 时，$P(S_z=-\frac{\hbar}{2})=\sin^2[\frac{\Omega_0t}{2}]=P(S_z=-\frac{\hbar}{2})_{max}$.

此时发生共振，能量最高

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微波激射.

在有势场中，含时方程 $i\hbar\frac{\partial}{\partial t}\psi=(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U)\psi=E\psi \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi=(E-U)\psi$

则对于 $\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$，本征能量为 $E-U$

在电场 ε 中存在氨分子偶极矩 P，$\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\pm\varepsilon P$（氨分子双态，对应 $\pm$）

$\therefore H=\begin{pmatrix} E-\varepsilon P & -A \\ -A & E+\varepsilon P\end{pmatrix}$，同前理，解得 $\cancel{E_{1,2}=E\pm A\pm\frac{\varepsilon^2P^2}{2A}}$

$$E_{1,2}=E\pm\sqrt{A^2+\varepsilon^2P^2}$$

本征矢不要求.

若用 ψ_1，ψ_2 展开，$|C_1|^2=\cos^2\frac{\sqrt{A^2+\varepsilon^2P^2}}{\hbar}t$，$|C_2|^2=\sin^2\frac{\sqrt{A^2+\varepsilon^2P^2}}{\hbar}t$.

例1 一维无限深势阱 $(0<x<a)$，自旋 $s=0$ 的两个粒子，不存在相互作用，写出体系最低的两个能级和波函数.

解：$E_n=n^2\frac{\pi^2\hbar^2}{2ma^2}$，$E=E_1+E_1=\frac{\pi^2\hbar^2}{ma^2}$，$\phi=\psi_1(x_1)\psi_1(x_2)$

$\psi_n=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$ $\qquad \phi=\frac{2}{a}\sin\frac{\pi x_1}{a}\sin\frac{\pi x_2}{a}$

实际上是 $\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}+(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2})$，$\hat{H}\phi=E\phi\Rightarrow\phi=\psi_1(x_1)\psi_1(x_2)$

当全同时，只有 $\phi=\psi_1(x_1)\psi_1(x_2)$ 才满足 $\hat{H}$ 的方程，又恰好全同交换后能量

$\phi'=\psi_1(x_2)\psi_1(x_1)=\phi$ 简并.

$E=E_1+E_2=\frac{5}{2}\frac{\pi^2\hbar^2}{ma^2}$，$\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}+-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2}$，此时为 ψ_1，ψ_2，不全同.

$\phi=\frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_2(x_2)+\psi_2(x_1)\psi_1(x_2))$，能量与 $\phi'=\frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_2(x_2)-\psi_1(x_2)\psi_2(x_1))$ 简并.