PHYS 621 Lecture Notes 5

N3.4 Ensembles and the density matrix

Quantum mechanical states $|\psi\rangle \in \mathcal{H}$ are called pure states.

↑ Hilbert space

We are often interested in an ensemble of states distributed with a classical probability distribution p_i that specifies the likelihood that an element of the ensemble will be found in the state $|i\rangle$.

← a state that the system might be found in

In this case we cannot describe the system by an element of the Hilbert space.

Instead we describe the system in terms of a density matrix $\hat{\rho}$ that acts on the Hilbert space:

$$\boxed{\hat{\rho} = \sum_i p_i |i\rangle\langle i|}$$

Average value of an observable $\hat{A}$:

$$\boxed{\langle \hat{A} \rangle = \sum_i p_i \langle i|\hat{A}|i\rangle}$$

Suppose the eigenstates of $\hat{A}$ are $|n\rangle$ with eigenvalues λ_n:

$$\hat{A}|n\rangle = \lambda_n|n\rangle.$$

Then $$\mathrm{Tr}(\hat{\rho}\hat{A}) = \sum_n \langle n|\hat{\rho}\hat{A}|n\rangle$$

$$= \sum_n \langle n| \underbrace{\sum_i p_i |i\rangle\langle i|}_{\hat{\rho}} \hat{A}|n\rangle$$

$$= \sum_n \sum_i p_i \langle n|i\rangle\langle i|n\rangle \lambda_n$$

$$= \sum_i p_i \sum_n |\langle i|n\rangle|^2 \lambda_n$$

$$= \sum_i p_i \sum_n \underbrace{\mathrm{prob}(n|i)}_{\text{probability of finding } \lambda_n \text{ given the state } |i\rangle} \lambda_n$$

$$= \sum_i p_i \langle\hat{A}\rangle_i$$

Average of $\hat{A}$ in state $|i\rangle$.

$$= \langle\hat{A}\rangle$$

$\Rightarrow$ The ensemble quantum average value of $\hat{A}$ is:

$$\boxed{\langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})}$$

$\sum_i p_i = 1$ (Sum of probabilities is 1)

$$\rightarrow \mathrm{Tr}\,\hat{\rho} = \mathrm{Tr}(\hat{\rho}\hat{\mathbb{1}}) = \sum_i p_i \langle\hat{\mathbb{1}}\rangle_i = \sum_i p_i = 1$$

$$\Rightarrow \boxed{\mathrm{Tr}\,\hat{\rho} = 1.}$$

For an ensemble consisting only of samples of the pure state $|\psi\rangle$,

$$P_\psi = 1$$ (probability of state $|\psi\rangle$ is 1.)

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

$$\langle \hat{A} \rangle = \mathrm{Tr}\, \hat{\rho} \hat{A} = \sum_n \langle n|\psi\rangle\langle\psi|\hat{A}|n\rangle$$

$$= \sum_n \langle n|\psi\rangle \langle\psi|n\rangle \lambda_n$$

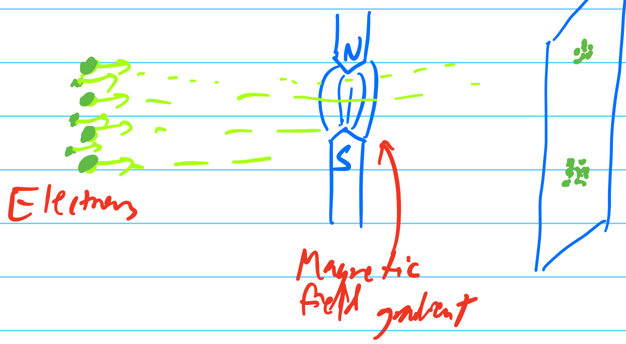
$$= \sum_n \underbrace{|\langle n|\psi\rangle|^2}_{\text{prob}(n|\psi)} \lambda_n$$

$$= \langle \hat{A} \rangle_\psi$$ the quantum-mechanical pure-state expectation value.

N3.1

Spin-½ Two-Level System (1922)

The Stern-Gerlach Experiment



$\uparrow \hat{z}$

magnetic moment of electron; Applied magnetic field.

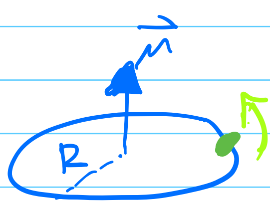
$$F_z = \frac{\partial}{\partial z}\left(\vec{\mu} \cdot \vec{B}(z)\right)$$

$$= \mu_z \frac{\partial B_z}{\partial z}$$

Classically, bending of trajectory of a magnet through a magnetic field depends on the magnetic moment and its orientation.

Experimentally, it appears that the component of the electron's magnetic moment about a given axis can only have two values, corresponding to the two clusters of electrons reaching the screen in the Stern-Gerlach Experiment.

Classically, $\mu \propto$ Angular Momentum:



charge; period of orbit

$$\text{Current } I = e/T = e \cdot v/2\pi R$$

$$\mu = |\vec{\mu}| = I \cdot \pi R^2$$

$$= \frac{e \cdot vR}{2} = \frac{e \cdot (mvR)}{2m}$$

$$= \frac{e}{2m} L$$

$L = |\vec{L}|$ angular momentum

For spin, $\vec{\mu}_s = g \frac{e}{2m} \vec{S}$

Landé g-factor $g \simeq 2$.

Write $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$

$$\Rightarrow \vec{\mu}_s = g \frac{e\hbar}{2m} \vec{\sigma}/2$$

Bohr magneton

$$\mu_B = \frac{e\hbar}{2m}$$

Electrons have spin angular momentum with observed

$$S_z = \pm \hbar/2$$

z-component of spin $\vec{S}$.

$\hbar$ = Planck's constant

Notation: $|\uparrow\rangle = |+\rangle = |S_z = +\frac{1}{2}\hbar\rangle$

$|\downarrow\rangle = |-\rangle = |S_z = -\frac{1}{2}\hbar\rangle$

Operators acting on the spin-1/2 system are represented by 2×2 matrices.

In the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis, $|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$

$\underline{S_z} \begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}$, $\quad \underline{S_z} \begin{pmatrix}0\\1\end{pmatrix} = -\frac{\hbar}{2}$

$S_z = +\hbar/2$ $\quad$ $S_z = -\hbar/2$

$$\underline{S_z} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Rightarrow \boxed{\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

What about components of spin about other axes?

– want $S_x^2 = S_y^2 = S_z^2 = \frac{\hbar^2}{4}\mathbb{1}$

<u>Later</u>: We will discuss rotations, which will be generated by the angular momentum operators.

$$\Rightarrow \begin{cases} \sigma_x\sigma_y - \sigma_y\sigma_x = i\sigma_z \\ \sigma_y\sigma_z - \sigma_z\sigma_y = i\sigma_x \\ \sigma_z\sigma_x - \sigma_x\sigma_z = i\sigma_y \end{cases}$$

Solution with $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$:

$$\boxed{\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}, \quad \boxed{\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}$$

Defining $(\sigma_1, \sigma_2, \sigma_3) = (\sigma_x, \sigma_y, \sigma_z)$,

the σ_i, $i \in \{1, 2, 3\}$, satisfy:

$$\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$$

Kronecker delta　　　Levi-Civita symbol

$$\epsilon_{ijk} = \begin{cases} +1 & \text{for } (ijk) = (123) \text{ and cyclic permutations (even)} \\ -1 & \text{for odd permutations} \\ 0 & \text{if any two of } i,j,k \text{ are equal} \end{cases}$$

ϵ_{ijk} is completely antisymmetric under exchange of 1,2,3 indices:

$$\epsilon_{ijk} = -\epsilon_{jik}, \text{ etc.}$$

Energy due to interaction of magnetic moment w/ magnetic field:

$$\Delta H_{spin} = -\vec{\mu}_s \cdot \vec{B}$$

$$= -\frac{ge\hbar}{4m}\vec{\sigma}\cdot\vec{B} = -\mu\,\vec{\sigma}\cdot\vec{B}$$

$$\mu = \frac{ge\hbar}{4m}$$

Suppose $\vec{B} = B_z\,\vec{e}_z$.

unit vector in z-direction

Then $\Delta H_{spin} = -\mu B_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Suppose $|\psi\rangle = |\uparrow\rangle$.

$$\Delta H_{spin}|\uparrow\rangle = -\mu B_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\mu B_z \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Similarly, $\Delta H_{spin}|\downarrow\rangle = +\mu B_z \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

→ $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of $\hat{S}_z$ with eigenvalues $\pm\frac{\hbar}{2}$, and eigenstates of ΔH_{spin} with eigenvalues $\mp \mu B_z$.

Consider the states $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix}$$

$$\text{prob}\left(S_z = +\tfrac{1}{2}\hbar\right) = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

$$\text{prob}\left(S_z = -\tfrac{1}{2}\hbar\right) = \left(\pm\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

Spin Energy: $|\psi_\pm\rangle$ is not an eigenstate of ΔH_{spin}, but we can calculate the average of ΔH_{spin}!

$$\langle \Delta H_{spin}\rangle = \langle \psi_\pm|(-\mu B_z \sigma_z)|\psi_\pm\rangle$$

$$= -\mu B_z \frac{1}{\sqrt{2}}(1, \pm 1)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix}$$

$$= -\mu B_z \cdot \frac{1}{2}(1, \pm 1)\begin{pmatrix}1\\ \mp 1\end{pmatrix}$$

$$= -\mu B_z \cdot \frac{1}{2}(1-1) = \boxed{0}$$