

SPUM 2018/202

APAC 4004 Mathematical method
of physics.

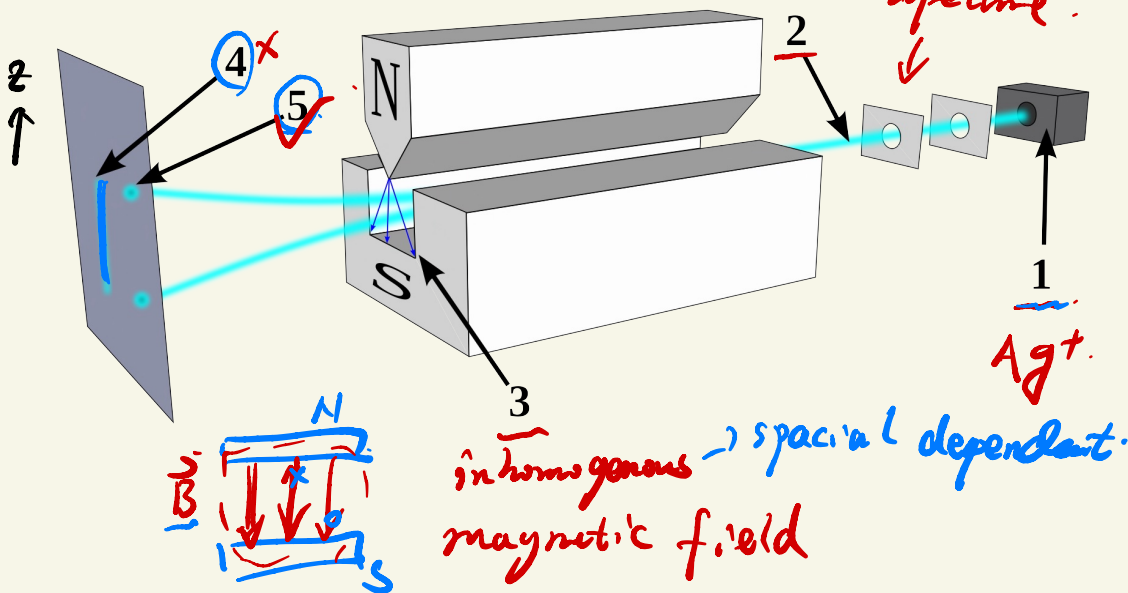
analytic solution \rightarrow numerical \sim

- Stern - Gerlach Experiment.


SG - experiment.

Ag: $[kr] 4d^{10} \underline{ss} \textcircled{1}$

\uparrow spin-up
 \downarrow spin-down
electron beam aperture.



1922. Walter Gerlach
 electrons have two spin states

 e^- magnetic moment. $\vec{\mu}$

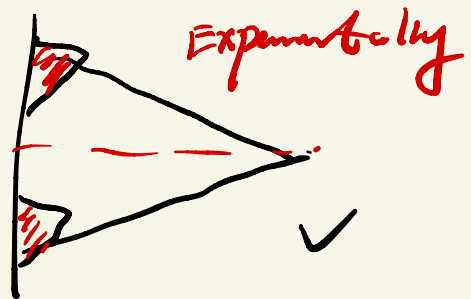
$$\vec{\mu} = -\frac{e}{mc} \cdot \vec{S} \rightarrow \text{spin}$$

$$\vec{F}_z = \frac{\partial}{\partial z} E.$$

$$= \frac{\partial}{\partial z} (-\vec{\mu} \cdot \vec{B})$$

$$= \left[\frac{e S_z}{mc} \cdot \frac{\partial B_z}{\partial z} \right] \quad \frac{\partial B_z}{\partial z} < 0$$

\vec{F}_z opposite to the spin of e^-



conclusion: e^- only has two spin states: S_{z+} or S_{z-} .

- Fundamental principles of QM.

\mathcal{H} , Hilbert space. 希尔伯特空间.

ket vector: $|a\rangle \in \mathcal{H}$.

bra vector: $\langle b| = (|b\rangle)^* \in \mathcal{H}$.

Inner product: $\langle a|b\rangle = \int a^* b d^3x$.

Basis: $\{|e_i\rangle\} \in \mathcal{H}$.

Complete Basis: $\forall |a\rangle \in \mathcal{H}, \exists c_i \in \mathbb{C}$

s.t. $|a\rangle = \sum_i c_i |e_i\rangle$.

α operators \hat{A} e.g. $\hat{A}\psi = -i\hbar \frac{\partial}{\partial x} \psi$.

observables: $\hat{H}, \hat{P}, \hat{L}, \dots$ $\hat{A}|a\rangle = |a'\rangle$
 $\{ = a_i |a\rangle$.

unitary operator: $\hat{A}^\dagger = \hat{A}^{-1}$, $e^{-\frac{i\hat{H}t}{\hbar}} \cdot e^{\frac{i\hat{H}t}{\hbar}} = I$

other operators: \hat{a}^\dagger, \hat{a} .

Fock state (number) state
 $\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$.

time evolution operator.

Example 1. $a^\dagger a = \hat{N}$ (Harmonic oscillator)

\hat{N} : number of particles.

$\hat{N}|n\rangle = n|n\rangle$. Phonons, b^\dagger, b .
photon, coherent state.

Example 2. \hat{H} . observable. $|\psi_i\rangle$ is time indep

$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$. Schrödinger's Eq.

Notice that $|\psi_i\rangle$ are eigenvectors of \hat{H}

— Inner product.

$\langle a|b\rangle \in \mathbb{C}$. $\langle a|b\rangle = (\langle b|a\rangle)^*$
bra ket

* Normalization.

$|a\rangle$. $\langle a|a\rangle \neq 1$. unnormalized.

$\langle a|a\rangle = \|a\|^2$; $\|a\|$, norm.

$|\bar{a}\rangle = \frac{1}{\sqrt{\langle a|a\rangle}} |a\rangle = \frac{|a\rangle}{\|a\|}$

$\langle \bar{a}|\bar{a}\rangle = \frac{\langle a|a\rangle}{\|a\|^2} = 1$

- Eigen vectors. as basis -

$$\hat{H} |\psi_i\rangle = E_i |\psi_i\rangle \quad [\text{Theorem 1.}]$$

$\{|\psi_i\rangle\}$ is a complete basis.

EX 3. $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$. $E_i = (n + \frac{1}{2}) \hbar \omega$

EX 4. Central potential. $\{|0\rangle, |1\rangle, |2\rangle, \dots\}$

$$V(r) = A \frac{1}{r}$$

$$\hat{H} |n, l, j, m_j\rangle = E_{nlj} |n, l, j, m_j\rangle$$

↓
Spherical Harmonics



$\{|a_i\rangle\}$ is a set basis in \mathcal{H} .

For $\forall |\alpha\rangle \in \mathcal{H}$.. how to describe $|\alpha\rangle$ in terms of $\{|a_i\rangle\}$?

$$|\alpha\rangle = \underline{c_0} |a_0\rangle + \underline{c_1} |a_1\rangle + \dots + \underline{c_n} |a_n\rangle$$

$$\langle a_i | a_j \rangle = \delta_{ij}$$

orthogonality:

$$C_i = \langle a_i | \alpha \rangle.$$

$$= \sum_{j=0}^n \langle a_i | c_j | a_j \rangle$$

$$= \sum_{j=0}^n c_j \langle a_i | a_j \rangle = \sum_{j=0}^n c_j \delta_{ij}.$$

$$= c_i.$$

so.

$$|\alpha\rangle = \sum_{i=0}^n c_i |a_i\rangle = \left(\sum_{i=0}^n |a_i\rangle \langle a_i| \right) |\alpha\rangle \quad \star$$

- completeness.

$$\{|a_i\rangle\} \quad \sum_{i=0}^n |a_i\rangle \langle a_i| = I \Leftrightarrow \{|a_i\rangle\} \text{ is complete}$$

- projection operator.

$$\hat{A}_{a_i} \equiv |a_i\rangle \langle a_i|.$$

1) completeness $\Leftrightarrow \sum_i \hat{A}_{a_i} = I$

2) expansion of $\forall |\alpha\rangle$: $|\alpha\rangle = \sum_{i=0}^n \hat{A}_{a_i} |\alpha\rangle$



Fundamental
principles

space, vector, basis, operators
linear product $\langle a|b \rangle$
superposition $|a\rangle = \sum c_i |a_i\rangle = \sum b_i |A_i\rangle$
Eigenvectors
matrix representation.
measurement, observables.

- Matrix representation

EX. 1
 $\hat{H} = \begin{bmatrix} \Omega & 0 \\ 0 & -\Omega \end{bmatrix} = \Omega \hat{\sigma}_z \rightarrow \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$|+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}^T, \quad |-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}^T$

$\hat{H} = \Omega |+\rangle\langle +| + (-\Omega) |-\rangle\langle -|$
 $= \begin{bmatrix} \Omega & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & \Omega \end{bmatrix} = \begin{bmatrix} \Omega & 0 \\ 0 & -\Omega \end{bmatrix}$

If $\{|a_i\rangle\}$ are eigenvectors of \hat{A} with corresponding eigenvalues λ_i , then \hat{A} is diagonalized.

$\hat{A} = \sum_i \lambda_i |a_i\rangle\langle a_i|$

Unluckily, \hat{A} is represented under.

$$\left\{ \begin{aligned} |a_0\rangle &= \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \end{bmatrix}^T, & |a_1\rangle &= \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \end{bmatrix}^T. \\ |a_2\rangle &= \begin{bmatrix} 0 & 0 & 1 & \dots & 0 \end{bmatrix}^T & \dots & |a_{n-1}\rangle &= \begin{bmatrix} 0 & 0 & 0 & \dots & 1 \end{bmatrix}^T \end{aligned} \right\}$$

$$\hat{A} = \sum_i \sum_j |a_i\rangle \langle a_i | \hat{A} | a_j \rangle \langle a_j | \quad (1)$$

$\langle a_i | \hat{A} | a_j \rangle = A_{ij}$: matrix element.

$$(1) \left\langle \hat{A} = \sum_i \sum_j A_{ij} |a_i\rangle \langle a_j| \right\rangle$$

EX 5-

$$\hat{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

$$= 1 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + 2 \cdot \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + 3 \cdot \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} + 4 \cdot \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= 1 \cdot \underbrace{\begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{|a_0\rangle} \underbrace{\begin{bmatrix} 1 & 0 \end{bmatrix}}_{\langle a_0|} + \dots + 4 \cdot \underbrace{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{|a_1\rangle} \underbrace{\begin{bmatrix} 0 & 1 \end{bmatrix}}_{\langle a_1|}$$

- Measurement; Observables. Uncertainty

$$(\Delta X)^2 (\Delta P)^2 \geq \frac{\hbar^2}{4}$$

You can not guarantee, that you probe. field will interact with your system.

* Observables.

classical mechanics: \vec{p}, E, \vec{L} : continuous.

QM. $\vec{p}, E, \vec{L}, \vec{S}$ are discrete quantities.
SG-experiment.

\hat{A} is an observable, then \hat{A} is Hermitian

$$\hat{A}^\dagger = (\hat{A}^*)^T = \hat{A}$$

$$(\hat{A} | \psi_i \rangle)^\dagger = (a_i | \psi_i \rangle)^\dagger \quad (2)$$

$$\langle \psi_i | \hat{A}^\dagger = \langle \psi_i | a_i$$

eigenvalues. $\in \mathbb{R}$.

$$\langle \vec{p} \rangle = \langle \psi | \hat{p} | \psi \rangle = \int \psi^* \hat{p} \psi d^3r.$$

sandwich.

EX6. probability density of states.

$$|\alpha\rangle = \sum_i c_i |a_i\rangle, \quad c_i \in \mathbb{C}.$$

observe $|\alpha\rangle$. What's the probability that

$|\alpha\rangle$ is at state $|a_i\rangle$

$$p(|\alpha\rangle = |a_i\rangle) = |c_i|^2 = c_i^* c_i$$

$\langle \hat{A}_{a_i} \rangle$ projection operator.

$$\hat{A}_{a_i} = |a_i\rangle \langle a_i|.$$

$$\begin{aligned} \langle \hat{A}_{a_i} \rangle &= \langle \alpha | \hat{A}_{a_i} | \alpha \rangle = \langle \alpha | a_i \rangle \langle a_i | \alpha \rangle \\ &= c_i^* c_i = |c_i|^2. \end{aligned}$$

ρ density operator (Density matrix)

$$\hat{\rho} \equiv |\alpha\rangle \langle \alpha| = \sum_i c_i \hat{A}_{a_i} \begin{bmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix}$$

A way to describe the probability distribution of the state.

- Compatible observables.

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}, \quad \text{Commutator.}$$

"对易括号"

$$\{A, B\} = \sum_i \left(\frac{\partial A}{\partial p_i} \frac{\partial B}{\partial z_i} - \frac{\partial B}{\partial p_i} \frac{\partial A}{\partial z_i} \right) \quad \text{Poisson Bracket}$$

if $[\hat{A}, \hat{B}] = [\hat{B}, \hat{A}] = 0$. \hat{A}, \hat{B} are commutative.
or (1) \hat{A}, \hat{B} are compatible.

"对易"

otherwise, (2) \hat{A}, \hat{B} are incompatible.

EX 7. Total Angular momentum. Hamiltonian.

$$\rightarrow H_{\uparrow}^{(0)} = \underbrace{\frac{p^2}{2m}}_{\text{kinetic}} - \underbrace{\left[\frac{1}{4\pi\epsilon_0} \frac{ze^2}{r} \right]}_{\text{central potential.}}$$

J^2 : total angular momentum.

$$[J^2, H^{(0)}] = 0, \quad [J^2, \underbrace{L^2}_{\text{orbital angular momentum}}] = 0$$

$$[J^2, \underbrace{J_z}_1] = 0$$

$H^{(0)}$ eigenstates. $\Leftrightarrow J^2, J_z, L^2$ eigenstates.

addition of
angular momentum.

$\bar{j}(j+1) \hbar^2$ $\bar{l}(l+1) \hbar^2$.

$$J^2 |n, l, j, m_j\rangle = \bar{j}(j+1) \hbar^2 |n, l, j, m_j\rangle$$

$$J_z |n, l, j, m_j\rangle = \hbar m_j |n, l, j, m_j\rangle.$$

separation of variables

$$L^2 |n, l, j, m_j\rangle = l(l+1) \hbar^2 |n, l, j, m_j\rangle.$$

$$H^{(0)} |n, l, j, m_j\rangle = E_n |n, l, j, m_j\rangle.$$

$$\rightarrow E_n = - \underbrace{\frac{1}{2} M c^2}_{\text{rest energy}} \underbrace{\alpha^2}_{\text{fine structure constant}} \underbrace{Z^2}_{\text{principal quantum number}} \frac{1}{n^2}$$

rest energy fine structure constant principal quantum number

$$= - \frac{e^2}{2a_0} \frac{1}{n^2}$$

\bar{a}_0 Bohr's radius.