Chap 9. Quantum Mechanical Description

9.0 Review on QM

9.0.1 Postulates of QM

- CM
  - state:
  - Dynamics:
- QM
  - Exist a state ftn $|\Psi\rangle$ s. t.
    -
    -
    - Hilbert space $\sim$ set of C-valued l^2 ftns
      $\sim$

- QM
  - Exist a state ftn $|\Psi\rangle$ ....
  - Exist a Hermitian (Self Adjoint) operator (observable) for each (measurable) physical quantity with

    CM :
    QM :
  - Measurement
    - measurement of an observable G
    -
  -

9.0.2 Representation (basis)

- Vectors in CM

$$\ddot{\vec{r}} =$$

$$\vec{v} =$$

$$=$$

- Representation

$$(\vec{v})_{\hat{x},\hat{y},\hat{z}} =$$

$$(\vec{v})_{\hat{x'},\hat{y'},\hat{z'}} =$$

- QM

Ex) Spin-1/2 system

- states :
  - $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ basis

    $(|\uparrow_z\rangle) \quad =$

    $(|\uparrow_x\rangle) \quad =$

  - $\{|\uparrow_x\rangle, |\downarrow_x\rangle\}$ basis

    $(|\uparrow_z\rangle) \quad =$

    $(|\uparrow_x\rangle) \quad =$

cf.
-
-

- Representation
  - Vector : The ith component is given by the left inner product with the ith basis vector, e. g., $v_i = \vec{a}_i \cdot \vec{v}$ or $\phi_i = \langle \alpha_i | \psi \rangle$ with basis sets $\{\vec{a}_i\}$ or $\{|\alpha_i\rangle\}$ respectively.
    - $(\vec{v})_{\{\vec{a}_1, \vec{a}_2\}}$
    - $(|\psi\rangle)_{\{|\alpha_1\rangle, |\alpha_2\rangle\}}$
  - Operator : The (i, j)th component of an operator A, A_{ij} is given by $A_{ij} = \langle \alpha_i | A | \alpha_j \rangle$ with a basis set $\{|\alpha_i\rangle\}$

    Example

    projection operator : $Pr_z = |\uparrow_z\rangle\langle\uparrow_z|$
    basis : $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ or $\{|\uparrow_x\rangle, |\downarrow_x\rangle\}$

$$(Pr_z)_{\{|\uparrow_z\rangle, |\downarrow_z\rangle\}} =$$

$$(Pr_z)_{\{|\uparrow_x\rangle, |\downarrow_x\rangle\}} =$$

- Inner product :
- Direct product:
- Representation for a direct product : $|\phi\rangle\langle\psi|$
  - $(A)_{ij} =$

    $(Pr_z) \quad =$
  - $(A) \ =$

    (Pr_z)
- Spectral decompositions of an Operator: $A = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$

Example: $s_z = \frac{\hbar}{2}(|\uparrow_z\rangle\langle\uparrow_z| - |\downarrow_z\rangle\langle\downarrow_z|)$

- $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ basis

  $(s_z) \ =$
- $\{|\uparrow_x\rangle, |\downarrow_x\rangle\}$ basis:

- Representation with a basis $\{|\alpha_i\rangle\}$
  - State (vector, Ray): $|\psi\rangle$
    $(|\psi\rangle) =$
  - Operator: $A = |\phi\rangle\langle\psi|$
    $(A) =$

    or a raw vector $(A)_i = \langle\alpha_i|\phi\rangle\langle\psi|$.
- Representation with a continous basis $\{|x\rangle\}$
  - state : $|\psi\rangle$
    x-components of $|\psi\rangle$:
  - operator p and x

$$\begin{aligned}
\langle x|p|x'\rangle &= \\
\langle x|x|x'\rangle &= \\
\langle x|p &= \\
\langle x|x &=
\end{aligned}$$

9.1 Density Operator

In MCE, probability that the system with enegery E in the state x is given by

- How do we discribe the system with $p(x) \ = \frac{1}{\Omega}\delta_{H(x),E}$ quantum mechanically?
- What is the meaning of $\delta_{H(x),E}$ when $H(x)$ is an operator?

• Consider a system described by a pure state, $|\psi\rangle$.
What is the meaning of $|\psi(x)|^2$?

-
- consider energy eigen state of free particle,

•

- How to discribe a system with fractional probability
- Density state (Density operator) formalism

A system which can be described by a pure state $|\psi\rangle$ is described by the density state

$$\rho = |\psi\rangle\langle\psi|$$

Density operator :

Density operator : semi-positive definite linear op. on $\mathbb{H}$ with $Tr\rho = 1$

• properties

- $Tr\rho =$
- $Tr\rho^2$
  - $Tr\rho^2 = 1$:
  - $Tr\rho^2 < 1$:
- $\langle G\rangle = Tr\rho G$
- $i\hbar\frac{d\rho}{dt} = [H\rho]$

Ex 1) Pure state ($Tr\rho^2 = 1$)

- $|\psi\rangle = |\uparrow_z\rangle \qquad \left[(|\psi\rangle) = (|\uparrow_z\rangle) = \begin{pmatrix}1\\0\end{pmatrix}\right]$

- $|\psi\rangle = |\uparrow_x\rangle \qquad \left[(|\psi\rangle) = (|\uparrow_x\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\right]$

Ex 2) Mixed state ($Tr\rho^2 < 1$)

- $\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$

- Partial trace

Classical (diagonalized) case

Ex 1) Two coins $\{(hh),(ht),(th),(tt)\}$

$$\rho = \begin{pmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix} \qquad P = \begin{pmatrix} 200 & 0 & 0 & 0 \\ 0 & 100 & 0 & 0 \\ 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\langle P \rangle = Tr\ \rho P = Tr \begin{pmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix} \begin{pmatrix} 200 & 0 & 0 & 0 \\ 0 & 100 & 0 & 0 \\ 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$= Tr \begin{pmatrix} 50 & 0 & 0 & 0 \\ 0 & 25 & 0 & 0 \\ 0 & 0 & 25 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = 50 + 25 + 25 = 100$$

- First coin $\rho_1 = Tr_2\ \rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$

Ex 2) Velocity distribution

$$\rho(\vec{q},\vec{p}) = e^{-\frac{\vec{p}^2}{2mT}}/(V/\lambda^3)$$

$$f(\vec{p}) = \frac{1}{h^3}\int d^3q\rho(\vec{q},\vec{p}) = Tr_q\ \rho(\vec{q},\vec{p})$$

- Partial trace

Ex) Two spin system (separable or entangled state)

- $$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow_1\uparrow_2\rangle + |\downarrow_1\downarrow_2\rangle)$$

$$\rho = |\psi\rangle\langle\psi|$$

$$\rho_1 =$$

$$(\rho_1) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \qquad (\rho_1^2) = \frac{1}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

cf.

$$(\langle\psi|) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix}$$

$$(\rho) = (|\psi\rangle)(\langle\psi|)$$

- $|\psi\rangle \;=\; \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle)$

$$(|\psi\rangle) \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix}$$

$$(\rho) \;=\; (|\psi\rangle)(\langle\psi|) \;=\; \frac{1}{2}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}(1,0,0,1) \;=\; \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix}$$

- cf. Tensor product in matrix form.

$$\begin{pmatrix}1 & 2\\3 & 4\end{pmatrix}\otimes\begin{pmatrix}2 & 1\\0 & 1\end{pmatrix} \;=$$

9.1.1 MCS

$$
\begin{aligned}
\rho &= \\
\Omega &= Tr\ \delta(H - E) \\
\rho_{mn} &=
\end{aligned}
$$

- delta ftn for operator
- matrix form of ρ
- Ω in matrix form

9.1.2 CS

$$\begin{aligned}\rho &= e^{-\beta H}/Tr\, e^{-\beta H}\\ Z &= Tr\, e^{-\beta H}\\ \langle G\rangle &= \frac{1}{Z} Tr\, e^{-\beta H} G\\ U &= \frac{1}{Z} Tr\, e^{-\beta H} H\\ S &= -\langle\, ln\rho\rangle\\ F &= U - TS\end{aligned}$$

matrix form

$$\rho_{m,n} = \langle m|\rho|n\rangle$$

9.1.3 GCS

$$\rho = \frac{e^{-\beta(H-\mu N)}}{Tr\ e^{-\beta(H-\mu N)}} = e^{-\beta(H-\mu N)}/Z_G$$

with $Z_G = Tr\ e^{-\beta(H-\mu N)}$.

Ex) Free Ptl

$$\begin{aligned}
H &= \\
H|\psi\rangle &= \\
\langle x|H|\psi\rangle &= \\
-\frac{\hbar^2}{2m}\nabla^2\psi(x) &= \\
\psi(x) &= \\
E &= \\
(k_x, k_y, k_z) &=
\end{aligned}$$

One free partile

$$
\begin{aligned}
Z(T,V,1) &= \\
&= \\
&= \\
&= \\
&= \\
&=
\end{aligned}
$$

where

$$\lambda = h/\sqrt{2\pi m T}$$

*momentum space representation

$$\rho_{\vec{k}'\vec{k}} =$$

*real space representation

$$\rho_{\vec{r}'\vec{r}} =$$

cf. $$\rho_u = e^{-\beta H}$$