第四章 表象与表象变换

单纯用Dirac表述过于抽象
能否用线性空间的构造来表示

$$|\psi\rangle = \sum C_n|\psi_n\rangle \Downarrow (C_1, C_2, \cdots, C_n)$$

1. 表象为量子态的表述方式

核心问题：
- 如何确定表象 ⟶ 如何确定展开的基
- 不同表象之间的关系 ⟶ 相同量子态在不同表象下的表示

2. 如何确定一组基

用力学量的本征态 ⟶ 正交归一完备的，且一般有可观测意义

a. 设 $\hat A$ 为力学量算符

如 $\hat A$ 的本征态均非简并 $\Longrightarrow$ ✓ 任意态均可用该基组展开，且基组由 $\hat A$ 的本征值唯一确定

如 $\hat A$ 的本征态有简并 $\Longrightarrow$ 对应 A_m 的 $|\psi_{m\alpha}\rangle$，构造两两正交的 $|\psi_{m\alpha}\rangle$

① 找到任一 $|\psi_{m1}\rangle$

② 构造与 $|\psi_{m1}\rangle$ 正交，且满足本征问题的态 $|\psi_{m2}\rangle$

③ 构造与 $\{|\psi_{m1}\rangle, |\psi_{m2}\rangle\}$ 正交 ······ $|\psi_{m3}\rangle$

······

④ 直到找不到为止，得到 s 个两两正交的本征态组成的简并子空间 (def)

prop. (i) $\hat A(\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle) = A_m(\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle)$

(ii) 子空间内任意态与本征值不为 A_m 的本征态正交 $\langle\psi_n|\sum_\alpha C_\alpha|\psi_{m\alpha}\rangle = 0$

(iii) 所有 $\hat A$ 的本征值为 A_m 的本征态都属于简并子空间

问题：由简并子空间多余的自由度导致无法由 $\hat A$ 的本征值唯一确定一组基

解决办法：找到一个合适的满足 $[\hat A, \hat B] = 0$ 的力学量 $\hat B$，由 $\hat B$ 在简并子空间内的非简并本征态唯一确定一组 $\{|\psi_{m\alpha}\rangle\}$

联合确定 $\begin{cases} \hat A|\psi_{m\alpha}\rangle = A_m|\psi_{m\alpha}\rangle \\ \hat B|\psi_{m\alpha}\rangle = B_m|\psi_{m\alpha}\rangle \end{cases}$

Thm：如 $[\hat A, \hat B] = 0$，则 $\hat A$，$\hat B$ 有共同本征态

证：(i) 对 $\hat A$ 的非简并本征态：$\hat B\hat A|\psi_n\rangle = \hat B A_n|\psi_n\rangle = \hat A\hat B|\psi_n\rangle \Longrightarrow \hat B|\psi_n\rangle = B_n|\psi_n\rangle$ 也是 $\hat B$ 本征态

$$0 = \langle\psi_n|[\hat A, \hat B]|\psi_k\rangle = \langle\psi_n|(\hat A\hat B - \hat B\hat A)|\psi_k\rangle = (A_n - A_k)\langle\psi_n|\hat B|\psi_k\rangle = 0$$

$$\Longleftrightarrow \langle\psi_n|\hat B|\psi_k\rangle = B_n\delta_{nk}$$

(ii) 对于简并子空间内的态

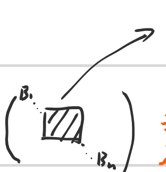
$\hat A\hat B|\psi_{m\alpha}\rangle = A_m\hat B|\psi_{m\alpha}\rangle \Longrightarrow \hat B|\psi_{m\alpha}\rangle$ 也在简并子空间内　$\hat B|\psi_{m\alpha}\rangle = \sum_{\alpha'} B_{\alpha\alpha'}|\psi_{m\alpha'}\rangle$

已知，可以实验上测

这矩阵 $(\langle\psi_{m\beta}|\hat B|\psi_{n\beta}\rangle)$

令 $|\psi\rangle = \sum_\alpha C_\alpha|\psi_{m\alpha}\rangle$ 求 C_α 使其满足 $\hat B|\psi\rangle = B|\psi\rangle$ （寻求通过前面来找到 $\hat B$ 的本征态）

$\hat B|\psi\rangle = \sum_{\alpha\alpha'} B_{\alpha\alpha'}C_\alpha|\psi_{m\alpha'}\rangle$　　$B|\psi\rangle = \sum_\alpha BC_\alpha|\psi_{m\alpha}\rangle$



矩阵非对角，下面求共同本征态的过程就是对角化过程

$\Rightarrow \sum_{\alpha\alpha'} B_{\alpha\alpha'} C_\alpha |\psi_{m\alpha'}\rangle = \sum_{\alpha'} B C_\alpha |\psi_{m\alpha'}\rangle$

$\xRightarrow{\langle\psi_{m\beta}|}$ $\sum_{\alpha\alpha'} B_{\alpha\alpha'} C_\alpha \delta_{\alpha'\beta} = \sum_{\alpha'} B C_{\alpha'} \delta_{\alpha'\beta}$ $(\ )(\ )=B(\ )$ → 本征值 → 本征向量

$\Rightarrow \sum_\alpha B_{\alpha\beta} C_\alpha = B C_\beta$ 本征线性方程组   有s组解，每组解给出 $B_m^{(\beta)}$ 及一组 $\{C_\alpha^{(\beta)}\}$

且有 $|\psi'_{m\beta}\rangle = \sum_\alpha C_\alpha^{(\beta)} |\psi_{m\alpha}\rangle$

ps: 这里的 $|\psi'_{m\beta}\rangle$ 是新的基.

则 $\hat A|\psi'_{m\beta}\rangle = A_m |\psi'_{m\beta}\rangle$ $\{|\psi'_{m\beta}\rangle\}$ 为共同本征基

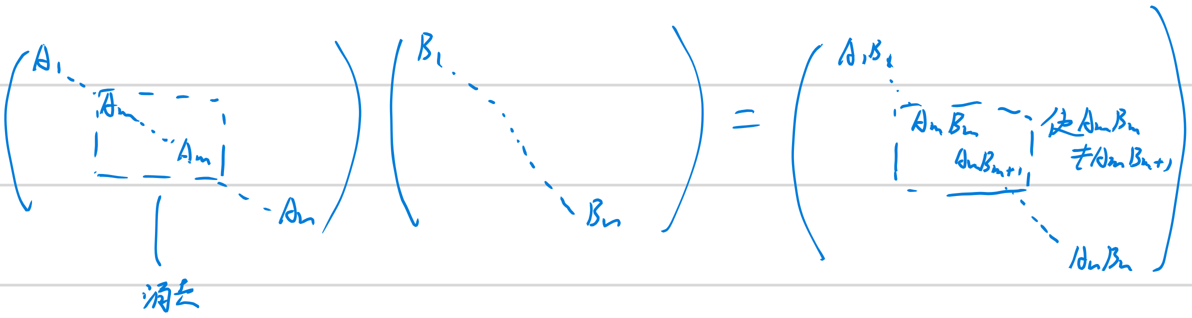
$\hat B|\psi'_{m\beta}\rangle = B_m^{(\beta)} |\psi'_{m\beta}\rangle$ □

即求C的本征问题.

ps: 若$\hat B$在$\hat A$简并子空间内仍简并，则引入第三个$\hat C$，有$[\hat A,\hat C]=[\hat B,\hat C]=0$，并在$\hat A\hat B$残余的简并子空间内继续对角化，直至共同本征态唯一标定

称$\{\hat A,\hat B,\hat C,\cdots\}$为体系的一个力学量完全集

矩阵诠释:



综上

$|\psi_1\rangle - - - |\psi_{m_1}\rangle \cdots |\psi_{m_s}\rangle - - - |\psi_n\rangle$

$A_1 - - - A_m \cdots A_m - - - A_n$

$A_1B_1 - - - A_mB_m \cdots A_mB_m \cdots A_nB_n$

$|\psi_1\rangle - - - |\psi'_{m_1}\rangle \cdots |\psi'_{m_2}\rangle \cdots |\psi_n\rangle$

非简并

此时力学量可唯一写成 $|\psi\rangle = \sum_{\alpha,\beta,\gamma\cdots} C_{\alpha,\beta,\gamma\cdots} |\alpha,\beta,\gamma,\cdots\rangle$

力学量完全集确定了一个表象，表象的基为完全集的共同本征态

例: 一维运动 $\{\hat x\}$ 与 $\{\hat p_x\}$ 都是力学量完全集

三维运动 $\{\hat x,\hat y,\hat z\}$ 与 $\{\hat p_x,\hat p_y,\hat p_z\}$ 都是力学量完全集

二维谐振子 $\{\hat N_x,\hat N_y\}$ 与 $\{\hat H,\hat N_x\}$ 都是力学量完全集 $\hat H=(\hat N_x+\hat N_y+1)\hbar\omega$

$|n_x,n_y\rangle$

3. 对易子，简并与量子涨落

Thm: 设 $[\hat A,\hat B]=0$ $\hat A|\psi_n\rangle = A_n|\psi_n\rangle$ 如 $\hat B|\psi_n\rangle \neq \overset{一个数}{B}|\psi_n\rangle$ 则 $|\psi_n\rangle$ 简并   (上面的推论)

Thm: 若 $[\hat A,\hat B]=0$ $[\hat A,\hat C]=0$ $[\hat B,\hat C]\neq 0$ 则$\hat A$的本征态存在简并

证: $\hat A|\psi_n\rangle = A_n|\psi_n\rangle$

$$\begin{cases} \hat A\hat B\hat C|\psi_n\rangle = A_n(\hat B\hat C|\psi_n\rangle) \\ \hat A\hat C\hat B|\psi_n\rangle = A_n(\hat C\hat B|\psi_n\rangle) \end{cases}$$

假设对$\forall|\psi_n\rangle$都不简并，则 $\hat B\hat C|\psi_n\rangle = k\hat C\hat B|\psi_n\rangle$

即 $\hat B\hat C = k\hat C\hat B$

由对称性 $k=1$ 违背$[\hat C,\hat B]\neq 0$

□

假设无简并

证2: $[\hat A,\hat B]=0$ $[\hat A,\hat C]=0$ $\Rightarrow$ $\hat B,\hat C$的本征态与$\hat A$相同

$\forall n$ $(\hat B\hat C-\hat C\hat B)|\psi_n\rangle = 0$ $\Rightarrow \forall|\psi\rangle$ $(\hat B\hat C-\hat C\hat B)|\psi_n\rangle = 0$ $\Rightarrow [\hat B,\hat C]=0$ 矛盾!

$\Delta A=\sqrt{\overline{(\hat{A}-\bar{A})^2}}=\sqrt{\langle\psi|\hat{A}^2|\psi\rangle-(\langle\psi|\hat{A}|\psi\rangle)^2}$ 若令 $\Delta A=0 \Leftrightarrow (\hat{A}-\bar{A})|\psi\rangle=0$ 即处于本征态时 $\Delta A=0$

广义不确定关系： $\Delta A\Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|$ (对易性在不确定性和共同本征态关系体现)

证：Schwarz不等式： 令 $|\alpha\rangle=(\hat{A}-\bar{A})|\psi\rangle$ $|\beta\rangle=(\hat{B}-\bar{B})|\psi\rangle$ $\langle\alpha|\alpha\rangle=\Delta A^2$ $\langle\beta|\beta\rangle=\Delta B^2$

$\langle\alpha|\beta\rangle=\langle\psi|(\hat{A}-\bar{A})(\hat{B}-\bar{B})|\psi\rangle$

$\Rightarrow \Delta A^2\Delta B^2 \geq |\langle(\hat{A}-\bar{A})(\hat{B}-\bar{B})\rangle|^2=|\langle\frac{1}{2}[\hat{A},\hat{B}]+\frac{1}{2}\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}\rangle|^2$

由 $[\hat{A},\hat{B}]^\dagger=\underset{反厄米}{-[\hat{A},\hat{B}]}$ $\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}^\dagger=\underset{厄米}{\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}}$

得 $\begin{cases}\langle[\hat{A},\hat{B}]\rangle^*=\langle[\hat{A},\hat{B}]^\dagger\rangle=-\langle[\hat{A},\hat{B}]\rangle & 即\langle[\hat{A},\hat{B}]\rangle 为纯虚数\\ \langle\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}\rangle 为实数\end{cases}$

$\Rightarrow \Delta A^2\Delta B^2 \geq \frac{1}{4}\left[|\langle[\hat{A},\hat{B}]\rangle|^2+|\langle\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}\rangle|^2\right] \geq \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2$

$\Rightarrow \Delta A\Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|$ □

故若 $[\hat{A},\hat{B}]=0$，则 $\Delta A=\Delta B=0$ 存在，即共同本征态存在

若 $[\hat{A},\hat{B}]\neq0$，$\Delta A,\Delta B$ 只在 $\langle[\hat{A},\hat{B}]\rangle=0$ 且 $\langle\{\hat{A}-\bar{A},\hat{B}-\bar{B}\}\rangle=0$ 时可以同时为0

4. 分离谱表象(矩阵表示)

设某力学量完全集定义了一组正交完备基 $\{|\psi_i\rangle\}$

$\begin{cases}\langle\psi_i|\psi_j\rangle=\delta_{ij}\\ \sum_i|\psi_i\rangle\langle\psi_i|=\hat{I}\end{cases}$ 体系任意态 $|\psi\rangle=\sum_i C_i|\psi_i\rangle$，则 $|\psi\rangle$ 在表象下的表示为 $\{C_i\}$ 或 $\begin{pmatrix}C_1\\ \vdots\\ C_n\end{pmatrix}$

相应的： $\langle\psi|=(|\psi\rangle)^\dagger$ 表示为 $(C_1^*,\cdots,C_n^*)$

$\langle\psi|\psi\rangle=(C_1^*,\cdots,C_n^*)\begin{pmatrix}C_1\\ \vdots\\ C_n\end{pmatrix}$ $(\vec{a}=A\vec{C})$

对于 $\hat{A}$： $A_{ij}=\langle\psi_i|\hat{A}|\psi_j\rangle$ $|\varphi\rangle=\hat{A}|\psi\rangle=\sum_{ij}A_{ij}C_j|\psi_j\rangle$ 设 $|\varphi\rangle=\sum_i a_i|\psi_i\rangle \Rightarrow a_i=\sum_j A_{ij}C_j$

即可以用矩阵表示 $\hat{A}$ (ps:矩阵一般是无穷维的，但实验上只关心一个小的子空间的有限维)

i) 算符不对易 ⟺ 矩阵不对易 ii) 算符本征问题 ⟺ 矩阵本征问题

prop. i) 算符在其本征态为基的表示下的矩阵为对角阵 $A_{ij}=\langle\psi_i|\hat{A}|\psi_j\rangle=A_j\delta_{ij}=A_i$

ii) 若一算符在某组基下的矩阵表示为对角阵，则该组基为其本征态，对角元为其本征值

$\hat{A}|\psi_i\rangle=\sum_j|\psi_j\rangle\langle\psi_j|\hat{A}|\psi_i\rangle=A_i|\psi_i\rangle$

(iii) 期望值

$\langle\psi|\hat{A}|\psi\rangle=\sum_{nm}\langle\psi|\psi_m\rangle\langle\psi_m|\hat{A}|\psi_n\rangle\langle\psi_n|\psi\rangle=\sum_{nm}C_m^*A_{mn}C_n=(\ \langle\psi|\ )\left(\ \hat{A}\ \right)\left(|\psi\rangle\right)$

如 A_{ij} 是对角阵，则 $\bar{A}=\sum_n|C_n|^2A_{nn}$

(iv) $\hat{A} = \sum_{ij} |\psi_i\rangle\langle\psi_i|\hat{A}|\psi_j\rangle\langle\psi_j| = \sum_{ij} A_{ij}|\psi_i\rangle\langle\psi_j|$

例: 正交归一完备的基组 $\{|1\rangle, |2\rangle\}$

$|1\rangle = 1\cdot|1\rangle + 0\cdot|2\rangle \rightarrow \begin{pmatrix}1\\0\end{pmatrix}$ $\quad |2\rangle = 0\cdot|1\rangle + 1\cdot|2\rangle \rightarrow \begin{pmatrix}0\\1\end{pmatrix}$

$\hat{A}|1\rangle = \alpha|1\rangle + \beta|2\rangle$ $\quad \hat{A}|2\rangle = \gamma|1\rangle + \lambda|2\rangle$ $\quad \Rightarrow \hat{A} \rightarrow \begin{pmatrix}\alpha & \gamma\\ \beta & \lambda\end{pmatrix}$

验证: $|1\rangle\langle 1| \Rightarrow \begin{pmatrix}1\\0\end{pmatrix}(1\ 0) = \begin{pmatrix}1&0\\0&0\end{pmatrix}$ $\quad |2\rangle\langle 2| \Rightarrow \begin{pmatrix}0&0\\0&1\end{pmatrix}$ $\quad |1\rangle\langle 2| \Rightarrow \begin{pmatrix}0&1\\0&0\end{pmatrix}$ $\quad |2\rangle\langle 1| \Rightarrow \begin{pmatrix}0&0\\1&0\end{pmatrix}$

$\Rightarrow \hat{A} = \sum_{ij} A_{ij}|\psi_i\rangle\langle\psi_j| = \alpha\left(\quad\right) + \beta\left(\quad\right) + \gamma\left(\quad\right) + \lambda\left(\quad\right)$ ✓

例: 本征问题 $\quad \hat{A} \Rightarrow \begin{pmatrix}1&1\\1&1\end{pmatrix}$ $\quad \lambda_1 = 0 \quad \lambda_2 = 2$ $\quad \cdots\cdots$ (跟LA完全一致)

归一化: $|\psi_{\lambda=0}\rangle = \frac{\sqrt{2}}{2}|1\rangle - \frac{\sqrt{2}}{2}|2\rangle$

$|\psi_{\lambda=2}\rangle = \frac{\sqrt{2}}{2}|1\rangle + \frac{\sqrt{2}}{2}|2\rangle$

例: 力学量完全集

设$\hat{A}$于基$\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle\}$下的矩阵表示为 $\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$ $\quad \begin{matrix}|\alpha\rangle & |\beta\rangle & |\gamma\rangle\\ \uparrow & \uparrow & \uparrow\\ 1, & -1, & -1\end{matrix}$ 是本征值

引入与$\hat{A}$对易的算符$\hat{B}$, 设其在基上的矩阵表示为 $\begin{pmatrix}2&0&0\\0&0&2i\\0&-2i&0\end{pmatrix}$ $\quad [\hat{A},\hat{B}]=0$

$|\alpha\rangle$是$\hat{B}$本征态, 但$|\beta\rangle$与$|\gamma\rangle$目前还不是(由于$\hat{A}$简并)

需在$\{|\beta\rangle, |\gamma\rangle\}$的子空间内对角化$\hat{B}$的矩阵

$\begin{pmatrix}0&2i\\-2i&0\end{pmatrix} \Rightarrow \begin{cases}\lambda = 2\\ \frac{\sqrt{2}}{2}\begin{pmatrix}1\\-i\end{pmatrix} \overset{\wedge}{\Rightarrow} |\beta'\rangle\end{cases}$ $\quad \begin{cases}\lambda = -2\\ \frac{\sqrt{2}}{2}\begin{pmatrix}1\\i\end{pmatrix} \overset{\wedge}{\Rightarrow} |\gamma'\rangle\end{cases}$

在$\{|\alpha\rangle, |\beta'\rangle, |\gamma'\rangle\}$基下

$\hat{A} \rightarrow \begin{pmatrix}1&&\\&-1&\\&&-1\end{pmatrix}$ $\quad \hat{B} \rightarrow \begin{pmatrix}2&&\\&2&\\&&-2\end{pmatrix}$

共同标定空间 $\quad |\alpha\rangle \triangleq |1,2\rangle \quad |\beta\rangle \triangleq |-1,2\rangle \quad |\gamma\rangle \triangleq |-1,-2\rangle$

5. 分离谱的表象变换

G表象: $\{|\psi_n\rangle\}$ 正交归一 $\qquad$ F表象: $\{|\psi_m\rangle\}$ 正交归一

对任意给定态$|\psi\rangle$ $\quad |\psi\rangle = \sum_n C_n|\psi_n\rangle = \sum_m C_m|\psi_m\rangle$

$\xrightarrow{\langle\psi_\beta|}$ $C_\beta = \sum_m \langle\psi_\beta|\psi_m\rangle C_m$ $\quad$ 定义 $S_{\beta m} = \langle\overset{\text{新基}}{\psi_\beta}|\overset{\text{旧基}}{\psi_m}\rangle$ 变换矩阵

$\Rightarrow C_\beta = \sum_m S_{\beta m}C_m$ $\quad (C') = (S)(C)$

prop. $(S^{+}S)_{mn}=\sum_{\beta}(S^{+})_{m\beta}S_{\beta n}=\sum_{\beta}S^{*}_{\beta m}S_{\beta n}=\sum_{\beta}\langle\psi_m|\underline{\psi_\beta\rangle\langle\psi_\beta|}\psi_n\rangle=\langle\psi_m|\psi_n\rangle=\delta_{mn}$

$\Rightarrow$ S 是幺正变换（正交变换，旋转空间，不改变模长），又是对称变换

对任意给定算符 $\hat{A}$:

$$A_{\alpha\beta}=\langle\psi_\alpha|\hat{A}|\psi_\beta\rangle=\sum_{mn}\langle\psi_\alpha|\psi_n\rangle\langle\psi_m|\hat{A}|\psi_n\rangle\langle\psi_n|\psi_\beta\rangle$$

$$=\sum_{mn}S_{\alpha m}A_{mn}S^{*}_{n\beta}$$

$$\Rightarrow A^{(F)}_{\alpha\beta}=\sum_{mn}(S)_{\alpha m}A^{(G)}_{mn}(S^{+})_{n\beta}\quad\Rightarrow\quad A^{(F)}=SA^{(G)}S^{+}$$

小结:	$\{\|\psi_n\rangle\}^{G}$ 表象		$\{\|\psi_n\rangle\}^{F}$ 表象
$\hat{A}\|\psi\rangle$	$A^{(G)}C^{(G)}$	一致性 $\Longleftrightarrow$	$A^{(F)}C^{(F)}=SA^{(G)}S^{+}SC^{(G)}=S(A^{(G)}C^{(G)})$
$\langle\varphi\|\hat{A}\|\psi\rangle$	$(a^{(G)})^{+}A^{(G)}C^{(G)}$		$(a^{(F)})^{+}A^{(F)}C^{(F)}=(Sa^{(G)})^{+}SA^{(G)}S^{+}(SC^{(G)})=(a^{(G)})^{+}A^{(G)}C^{(G)}$

$\downarrow$

可观测量与
表象无关（客观要求）

例：算符 $\hat{A}$ 在某基下的表示为 $\begin{pmatrix}1&1\\1&1\end{pmatrix}$，求其在 $\hat{A}$ 本征态基下的表示

$\begin{cases}\lambda_1=0\\|\psi_1\rangle=\frac{\sqrt2}{2}\begin{pmatrix}1\\-1\end{pmatrix}\end{cases}$ $\begin{cases}\lambda_2=2\\|\psi_2\rangle=\frac{\sqrt2}{2}\begin{pmatrix}1\\1\end{pmatrix}\end{cases}$ 变换矩阵: $S=\begin{pmatrix}\frac{\sqrt2}{2}(1\ -1)\begin{pmatrix}1\\0\end{pmatrix} & \frac{\sqrt2}{2}(1\ -1)\begin{pmatrix}0\\1\end{pmatrix}\\ \frac{\sqrt2}{2}(1\ 1)\begin{pmatrix}1\\0\end{pmatrix} & \frac{\sqrt2}{2}(1\ 1)\begin{pmatrix}1\\0\end{pmatrix}\end{pmatrix}=\begin{pmatrix}\frac{\sqrt2}{2}&-\frac{\sqrt2}{2}\\ \frac{\sqrt2}{2}&\frac{\sqrt2}{2}\end{pmatrix}$

$$A^{(F)}=SA^{(G)}S^{+}=\frac{1}{2}\begin{pmatrix}1&-1\\1&1\end{pmatrix}\begin{pmatrix}1&1\\1&1\end{pmatrix}\begin{pmatrix}1&1\\-1&1\end{pmatrix}=\begin{pmatrix}0&0\\0&2\end{pmatrix}$$

ps：注意以 $S^{+}=(\vec{x}_1,\vec{x}_2,\cdots,\vec{x}_n)$

例. $f(\hat{A})=\sum_{n}\frac{f^{(n)}(0)}{n!}\hat{A}^{n}\longrightarrow f(A^{(F)})=\sum_{n}\frac{f^{(n)}(0)}{n!}(A^{(F)})^{n}=Sf(A^{(G)})S^{+}$

由于 $e^{\begin{pmatrix}a&0\\0&b\end{pmatrix}}=\begin{pmatrix}e^{a}&0\\0&e^{b}\end{pmatrix}$，所以可将 $A^{(G)}$ 对角化成 $A^{(F)}$，就比较好算

6. 连续谱表象

def：当表象的基对应的力学量本征值可以连续取值时，称之为连续谱表象

$\begin{cases}\text{坐标表象}\ \{|r\rangle\}\\ \text{动量表象}\ \{|p\rangle\}\end{cases}$

a. 坐标表象 $\{|r\rangle\}$

$|\psi\rangle=\int d^3r\,|r\rangle\langle r|\psi\rangle=\int d^3r\,\psi(r)|r\rangle$

$\begin{cases}\int dr^3|r\rangle\langle r|=\hat{I}\\ \langle r|r'\rangle=\delta(r-r')\end{cases}$ → 奇性性质是因为 $|r\rangle$ 现实中不存在

* 连续谱表象的归一化：

$\langle\psi_m|\psi_n\rangle=\delta_{mn}$ $\langle\psi_m|\psi_n\rangle=\int d^3r\,d^3r'\langle\psi_m|r'\rangle\langle r'|r\rangle\langle r|\psi_n\rangle=\int d^3r\,d^3r'\,\psi^{*}_m(r)\langle r'|r\rangle\psi_n(r)$ 要求 $m=n$ 为1，只有使 $\langle r'|r\rangle=\delta(r'-r)$

* $\langle\varphi|\psi\rangle=\int d^3r\,\varphi^{*}(r)\psi(r)$

*算符的表示

$\hat{A}|\psi\rangle = |\varphi\rangle \quad \Rightarrow \quad \hat{A}|\psi\rangle = \int d^3r\, d^3r'\, |r\rangle\langle r|\hat{A}|r'\rangle\langle r'|\psi\rangle = \int d^3r\, \langle r|\varphi\rangle |r\rangle$

$\Rightarrow \quad \int d^3r'\, \langle r|\hat{A}|r'\rangle\, \psi(r') = \varphi(r)$

ex. $\langle r|\hat{r}|r'\rangle = r\delta(r-r') \qquad \langle r|V(\hat{r})|r'\rangle = V(r)\delta(r-r')$

* 问: $\langle r|\hat{p}|r'\rangle = ???$

一维情况: $\langle x|[\hat{x},\hat{p}]|x'\rangle = \langle x|\hat{x}\hat{p}-\hat{p}\hat{x}|x'\rangle = (x-x')\langle x|\hat{p}|x'\rangle = i\hbar\,\delta(x-x')$

考虑 $\int f(x)\delta'(x)\,dx = -\int f'(x)\delta(x)dx \overset{积分性质相同}{\Longleftrightarrow} f(x)\delta'(x) = -f'(x)\delta(x) \xRightarrow{取f(x)=x} x\delta'(x) = -\delta(x)$

$\xRightarrow{代入} \langle x|\hat{p}|x\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x')$

三维情况: $\langle r|\hat{p}|r'\rangle = -i\hbar\nabla_r\delta(r-r')$ $\quad \xRightarrow{外推}$ 若 $\hat{A} = A(\hat{r},\hat{p})$, 则 $\langle r|\hat{A}|r'\rangle = A(r, -i\hbar\nabla_r)\delta(r-r')$

讨论:

i) $\begin{cases} \langle x|\hat{p}|p\rangle = p\langle x|p\rangle \\ \langle x|\hat{p}|p\rangle = \int dx'\langle x|\hat{p}|x'\rangle\langle x'|p\rangle = \int dx'\left(-i\hbar\frac{\partial}{\partial x}\delta(x-x')\right)\langle x'|p\rangle = \int dx'\, i\hbar\frac{\partial}{\partial x'}\delta(x-x')\langle x'|p\rangle = -i\hbar\int dx'\,\delta(x-x')\frac{\partial}{\partial x}\langle x|p\rangle \\ \qquad = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle \end{cases}$

$\Rightarrow p\langle x|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle \quad \Rightarrow \quad \langle x|p\rangle \propto e^{\frac{ipx}{\hbar}} \qquad \langle r|p\rangle \propto e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}}$

ii) $\left(\psi(r) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int\varphi(p)\, e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}}\, d^3p\right) \qquad \langle r|\psi\rangle = \int d^3p\,\langle r|p\rangle\langle p|\psi\rangle \Rightarrow \langle r|p\rangle = \frac{e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}}}{(2\pi\hbar)^{\frac{3}{2}}} \Leftarrow$

$\langle r|r'\rangle = \int\langle r|p\rangle\langle p|r'\rangle d^3p$

$\boxed{\begin{aligned} &= \frac{1}{(2\pi\hbar)^3}\int e^{i\vec{p}(\vec{r}-\vec{r}')/\hbar}d^3p \\ &= \delta(r-r') \end{aligned}}$

(iii) $\langle r|\hat{p}|r'\rangle = \int d^3p\,\langle r|\hat{p}|p\rangle\langle p|r'\rangle = \int d^3p\,\vec{p}\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}e^{i\vec{p}\cdot\frac{(\vec{r}-\vec{r}')}{\hbar}} = -\frac{i\hbar}{(2\pi\hbar)^3}\nabla_r\int d^3p\, e^{i\vec{p}\cdot\frac{(\vec{r}-\vec{r}')}{\hbar}} = -i\hbar\nabla_r\delta(r-r')$

(iv) $\langle r|\hat{\vec{L}}|r'\rangle = -i\hbar\vec{r}\times\nabla_r\delta(r-r') \qquad \langle r|A(\hat{p})|r'\rangle = A(-i\hbar\nabla_r)\,\delta(r-r')$

$\langle r|\hat{H}|r'\rangle = -\frac{\hbar^2}{2m}\nabla^2\delta(r-r') + V(r)\delta(r-r')$

* Schrodinger 方程 (基本假设)

$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$

$\hat{H}|\psi\rangle = E|\psi\rangle \Rightarrow \langle r|\left[\frac{\hat{p}^2}{2m}+V(\hat{r})\right]|\psi\rangle = E\langle r|\psi\rangle \Rightarrow \int d^3r'\,\langle r|\left[\frac{\hat{p}^2}{2m}+V(\hat{r})\right]|r'\rangle\langle r'|\psi\rangle = E\langle r|\psi\rangle$

$\Rightarrow \int d^3r'\left[\frac{(-i\hbar\nabla)^2}{2m}\delta(r-r') + V(r)\delta(r-r')\right]\psi(r) = E\psi(r) \Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\psi(r)$

连续谱 $\Rightarrow i\hbar\frac{\partial}{\partial t}\langle r|\psi\rangle = \int d^3r'\,\langle r|\hat{H}|r'\rangle\langle r'|\psi\rangle$

$\Rightarrow i\hbar\frac{\partial}{\partial t}\psi(r) = \int d^3r'\left[-\frac{\hbar^2}{2m}\nabla^2\delta(r-r') + V(r)\delta(r-r')\right]\psi(r')$

$\Rightarrow i\hbar\frac{\partial}{\partial t}\psi(r) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r)$

分立谱: $i\hbar\frac{\partial}{\partial t}\langle\psi_n|\psi\rangle = \sum_m\langle\psi_n|\hat{H}|\psi_m\rangle\langle\psi_m|\psi\rangle$

$\Rightarrow i\hbar\frac{\partial}{\partial t}C_n = \sum_m H_{nm}C_m$

(v) 期望值

$\langle\psi|\hat{A}|\psi\rangle = \int d^3r\, d^3r'\,\psi^*(r)\,\langle r|\hat{A}|r'\rangle\,\psi(r') = \int d^3r\;\psi^*(r)\,A(r, -i\hbar\nabla_r)\,\psi(r)$

6. 动量表象

$|\psi\rangle = \int d^3p\, \varphi(p)\, |p\rangle$

$\langle p|\hat{p}|p'\rangle = p\,\delta(p-p')$

$\langle p|A(\hat{p})|p'\rangle = A(p)\,\delta(p-p')$

$$\langle p|\hat{r}|p'\rangle = \int d^3r\, d^3r' \langle p|r\rangle\langle r|\hat{r}|r'\rangle\langle r'|p'\rangle$$
$$= \int d^3r\, \vec{r}\, \langle p|r\rangle\langle r|p'\rangle$$
$$= \frac{1}{(2\pi\hbar)^3}\int d^3r\,(i\hbar\nabla_p)\, e^{i\frac{(\vec{p}'-\vec{p})\cdot\vec{r}}{\hbar}}$$
$$= i\hbar\nabla_p\, \delta(p-p')$$

7. 连续谱的表象变换

$\{|r\rangle\} \longrightarrow \{|p\rangle\}$ Fourier 变换

① $|\psi\rangle = \int d^3r\, \psi(r)\,|r\rangle = \int d^3p\, \varphi(p)\,|p\rangle$

$\overset{\langle r'|}{\Longrightarrow}$ $\psi(r') = \int d^3p\, \varphi(p)\langle r'|p\rangle = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int d^3p\, \varphi(p)\, e^{i\frac{\vec{p}\cdot\vec{r}'}{\hbar}}$

② $\langle r|\hat{A}|r'\rangle = \int \underset{\sim}{\langle r|p\rangle}\langle p|\hat{A}|p'\rangle\underset{\sim}{\langle p'|r'\rangle}\, d^3p\, d^3p'$

连续谱 ⟺ 分离谱：

$|\psi\rangle = \sum_n C_n|\psi_n\rangle$

变换阵

① $\begin{cases} C_n = \langle\psi_n|\psi\rangle = \int d^3r\, \langle\psi_n|r\rangle\langle r|\psi\rangle = \int d^3r\, \psi_n^*(r)\,\psi(r) \\ \psi(r) = \langle r|\psi\rangle = \sum_n \langle r|\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n \psi_n(r)\, C_n \end{cases}$

② $A_{mn} = \langle\psi_m|\hat{A}|\psi_n\rangle = \int d^3r\, d^3r'\, \langle\psi_m|r\rangle\langle r|\hat{A}|r'\rangle\langle r'|\psi_n\rangle = \int d^3r\, d^3r'\, \psi_m^*(r)\,\langle r|\hat{A}|r'\rangle\,\psi_n(r')$

关于 $\psi_n(r)$ 的讨论

$|\psi_n\rangle$ 的波函数 $\psi_n(r) = \langle r|\psi_n\rangle$

$\begin{cases} \langle\psi_n|\psi_m\rangle = \delta_{nm} \\ \sum_n \langle\psi_n|\psi_n\rangle = \hat{I} \end{cases} \Longrightarrow \begin{cases} \int d^3r\, \langle\psi_n|r\rangle\langle r|\psi_m\rangle = \int d^3r\, \psi_n^*(r)\,\psi_m(r) = \delta_{nm} \\ \sum_n \langle r|\psi_n\rangle\langle\psi_n|r'\rangle = \delta(r-r') \end{cases}$

$\{|\psi_n\rangle\} \Longrightarrow \{\psi_n(r)\}$ 函数空间的正交归一完备性

$\psi(r) = \langle r|\int d^3r \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle$
$= \sum_n \int d^3r\, \psi_n(r)\, C_n$

例：$e^{i\hat{p}a/\hbar}|\psi\rangle$ → 平移算符

坐标表象下： $\langle x|e^{i\hat{p}a/\hbar}|\psi\rangle = \int dx' \langle x|e^{i\frac{\hat{p}a}{\hbar}}|x'\rangle\langle x'|\psi\rangle$

$= \int dx'\, e^{i(-i\frac{\partial}{\partial x})a}\, \delta(x-x')\,\psi(x')$

$$= e^{a\frac{\partial}{\partial x}}\psi(x)$$

$$= \sum_{n} \frac{1}{n!} a^{n} \frac{\partial^{n}}{\partial x^{n}} \psi(x) = \psi(x+a)$$