量子力学形式理论

  

1926 - 1927

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为什么要研究抽象理论?

- ☒ 波动力学仅限于描述空间中运动的粒子（坐标或动量）
- ☒ 量子描述并不是独一无二的（坐标表象和动量表象给出一致结果）
- ☒ 但有许多物理量无法用坐标(x)和动量(p)来描述

例如：费米子自旋，强子同位旋，弱同位旋，夸克的色空间

抽象理论可以帮助我们更好地理解量子力学

Plancherel定理

两个波函数的如下积分和它们傅里叶变换后波函数的积分相等

$$\int \psi_1^*(\vec{r},t)\psi_2(\vec{r},t)d^3r = \int \varphi_1^*(\vec{p},t)\varphi_2(\vec{p},t)d^3p$$

$$(\psi_1(\vec{r},t),\psi_2(\vec{r},t)) = (\varphi_1(\vec{p},t),\varphi_2(\vec{p},t))$$

数学家理解上面等式背后的结构：

这些积分是两个复函数的标量内积

例：有限维复向量空间—厄米空间

简单起见，考虑二维空间，

矢量 $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ 共轭矢量 $\bar{u} = \begin{pmatrix} u_1^* & u_2^* \end{pmatrix}$

厄米标量积 $(v, u) = v_1^* u_1 + v_2^* u_2$

矢量模 $||u|| = (u, u) \geq 0$

矩阵的厄米共轭 $M_{ij}^\dagger = (M_{ji})^*$

厄米矩阵 $M^\dagger = M$

厄米矩阵的本征值是实数，其归一化的本征向量构成了厄米空间的正交归一的基矢

例：平方可积复函数的向量空间

与量子力学紧密相关的是平方可积函数：满足如下条件的实变量的复函数

$$\int_{-\infty}^{+\infty} |f(x)|^2 dx < \infty$$

数学上将平方可积函数的集合即作为 $\mathcal{L}^2(R)$，所以$f \in \mathcal{L}^2(R)$

线性代数：平方可积函数的集合构成一个复向量空间V

这个集合中元素之间可以定义加法“+”，同时也可以定义它的一个元素和一个复数的数乘，这些操作之间满足分配律

可证：任何平方可积函数的线性组合仍然是平方可积的，即V对于上述加法和数乘运算是封闭的。

例：平方可积复函数的向量空间

任取 $\mathcal{L}^2(R)$ 上的函数 $f(x)$ 和 $g(x)$，则它们任何一个线性组合

$G(x) = af(x) + bg(x)$ 也是平方可积的。

$$\int_{-\infty}^{+\infty} |G(x)|^2 dx = \int_{-\infty}^{+\infty} |af(x) + bg(x)|^2 dx$$

$$= |a|^2 \int_{-\infty}^{+\infty} |f(x)|^2 dx + |b|^2 \int_{-\infty}^{+\infty} |g(x)|^2 dx + a^* b \int_{-\infty}^{+\infty} f^*(x) g(x) dx + ab^* \int_{-\infty}^{+\infty} f(x) g^*(x) dx$$

$$\leq |a|^2 \int_{-\infty}^{+\infty} |f(x)|^2 dx + |b|^2 \int_{-\infty}^{+\infty} |g(x)|^2 dx + 2|ab| \sqrt{\int_{-\infty}^{+\infty} |f(x)|^2 dx} \sqrt{\int_{-\infty}^{+\infty} |g(x)|^2 dx}$$

$$< \infty$$

其中用到Cauchy-Schwartz不等式：

$$\int_{-\infty}^{+\infty} f^*(x) g(x) dx \leq \sqrt{\int_{-\infty}^{+\infty} |f(x)|^2 dx} \sqrt{\int_{-\infty}^{+\infty} |g(x)|^2 dx}$$

Schwarz不等式

如果 ψ_1, ψ_2 是任意两个平方可积函数，则有

$$(\psi_1, \psi_1)(\psi_2, \psi_2) \geq |(\psi_1, \psi_2)|^2$$

证：令 $$\psi_3 = \psi_2 - \psi_1 \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)}$$

$$(\psi_3, \psi_3) = \left(\psi_2 - \psi_1 \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)}, \psi_2 - \psi_1 \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)} \right) \geq 0$$

得

$$(\psi_2, \psi_2) - (\psi_2, \psi_1)\frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)} - \frac{(\psi_1, \psi_2)^*}{(\psi_1, \psi_1)}(\psi_1, \psi_2)$$
$$+ \left(\frac{(\psi_1, \psi_2)^*}{(\psi_1, \psi_1)} \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)} (\psi_1, \psi_1) \right) \geq 0$$

从而证得：

$$(\psi_1, \psi_1) \cdot (\psi_2, \psi_2) \geq |(\psi_2, \psi_1)|^2$$

类似于

$$|\vec{A} \cdot \vec{B}|^2 \leq |\vec{A}|^2 |\vec{B}|^2$$

1. 平方可积函数的向量空间和量子力学的联系

Charles Hermite

1860年厄米研究复变函数性质时

定义了两个函数的厄米标量内积

$$(g, f) = \int g^*(x) f(x) dx$$

厄米标积满足厄米对称性

$$(g, f) = (f, g)^*$$

我们可以定义函数的Norm

$$||f||^2 = \int |f(x)|^2 dx$$

这和有限维向量空间的数学形式没有区别，虽然收敛性不同。

简谐振子本征值

厄米研究了简谐振子本征值问题

$$\hat{h}\varphi_n(x) \equiv \left(x^2 - \frac{d^2}{dx^2}\right)\varphi_n(x) = \varepsilon_n\varphi_n(x)$$

得到了离散的本征值和相应的平方可积的本征解

$$\varepsilon_n = 2n+1, \quad n = 0, 1, 2, \cdots$$

$$\varphi_n(x) = \gamma_n e^{x^2/2}\frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

归一化因子 $\gamma_n = \pi^{-1/4}2^{-n/2}(n!)^{-1/2}$

厄米函数 $\varphi_n(x)$ 是正交归一的，构成一组正交基

厄米的重要发现

所有平方可积函数都可以写作厄米函数的集合

$$\forall f \in \mathcal{L}^2(\mathcal{R}) \;, \quad f(x) = \sum_{n=0}^{\infty} C_n \varphi_n(x)$$

其中 $C_n = (\varphi_n, f)$

换言之，厄米函数构成一个完备集合，被称作 $\mathcal{L}^2(\mathcal{R})$ 的Hilbert基。

取厄米函数为基时，函数*f(x)*完全由它展开系数确定

$$f(x) \Leftrightarrow \{C_n\}$$

希尔伯特空间$\mathcal{H}$

平方可积复函数

$$\int_{-\infty}^{+\infty} |f(x)|^2 \, dx < \infty$$

构成的向量空间$L^2(R)$ $\quad x \in \Re$

* 独立性和完备性

矢量空间维数$d_V =$最大独立矢量的个数

厄米函数构成Hilbert基是无穷维的

取厄米函数为基时，函数f(x)完全由它展开系数确定

$$f(x) \Leftrightarrow \{C_n\}$$

我们可以“忘掉”厄米函数基，直接和展开系数打交道。例如，

$$f(x) = \sum_{n=0}^{\infty} C_n \varphi_n(x) \qquad g(x) = \sum_{n=0}^{\infty} B_n \varphi_n(x)$$

f(x)和g(x)的内积

$$(g, f) = \sum B_n^* C_n$$

$$||f||^2 = \sum |C_n|^2$$

Bessel-Parseval定理

能量平均值

$$\hat{h} f(x) = \sum C_n \hat{h} \varphi_n(x) = \sum C_n \varepsilon_n \varphi_n(x)$$

$$(f, \hat{h} f(x)) = \sum \varepsilon_n |C_n|^2$$

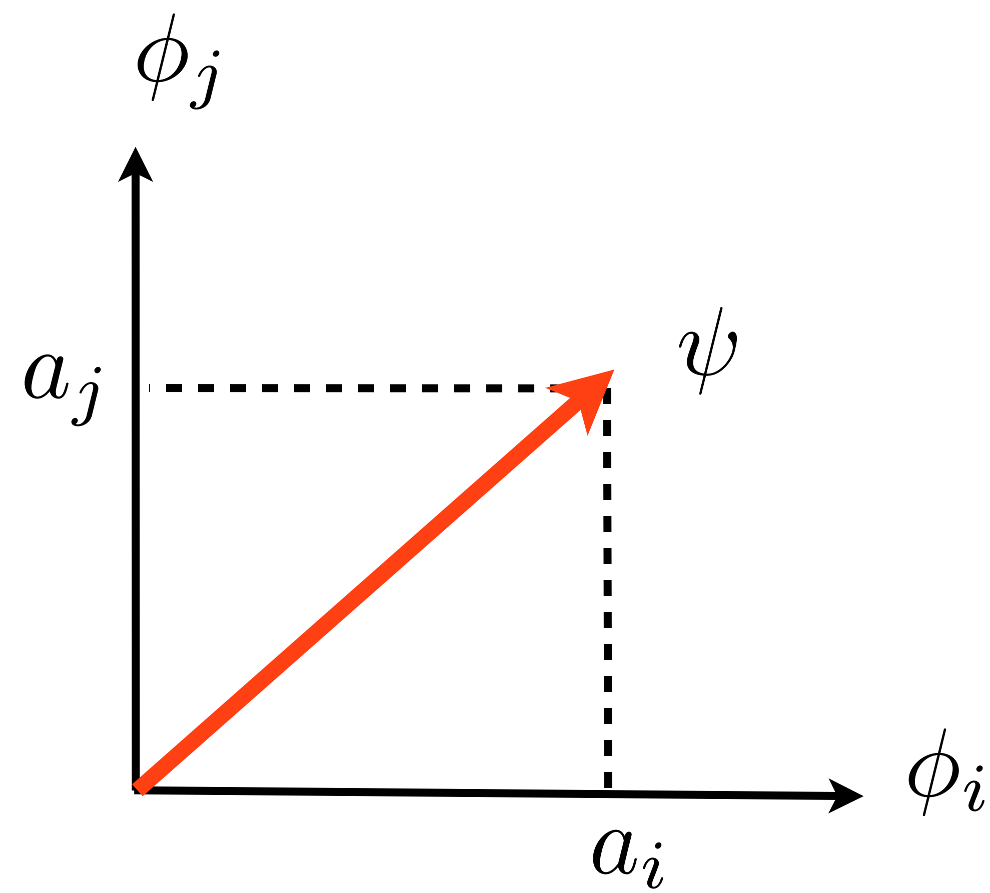
Hilbert空间的几何性质

矢量表示

$$\psi = \sum_{i=1}^{N} a_i \phi_i$$

$$a_j = \frac{(\phi_j, \psi)}{(\phi_j, \phi_j)}$$

$$\psi = \sum_j \frac{(\phi_j, \psi)}{(\phi_j, \phi_j)} \phi_j$$



矢量内积

$$(\psi, \psi') = \sum_{ij} \frac{(\phi_j, \psi)^*(\phi_i, \psi')}{(\phi_j, \phi_j)(\phi_i, \phi_i)} (\phi_j, \phi_i) = \sum_i \frac{(\phi_i, \psi)^*(\phi_i, \psi')}{(\phi_i, \phi_i)}$$

Hilbert空间的维数

（有限维 或 无限维）

无限维独立矢量集合的完备性

给定任一态矢量 ψ，总可以找到一组数 a_i 使得

$$\sum_{i=1}^{\infty} a_i \phi_i \to \psi$$

数学上，定义 $\Omega_N \equiv \psi - \sum_{i=1}^{\infty} a_i \phi_i$，当 $N \to \infty$ 时，

$$\langle \Omega_N | \Omega_N \rangle \to 0$$

这使得我们可以将无限维的希尔伯特空间视作为有限维来做同样的数学处理

波函数——态矢量

薛定谔波动力学中波函数 $\psi(\vec{r},t)$ 属于希尔伯特空间。

例：3维空间中的运动粒子的Hilbert空间是 $\mathcal{L}^2(R^3)$。

$R^3=(x,y,z)$

$\psi(\vec{r},t)$ 和 $\varphi(\vec{p},t)$ 是3维粒子运动的两种等价描述

$\longrightarrow$ 存在无穷多的等价描述。

采用抽象的Hilbert空间中的矢量 $\psi(t)$ 来描述物理体系的量子状态，不在拘泥于具体的表示空间。

$|\psi(t)\rangle \longrightarrow$ Hilbert空间的元素

量子力学第I条假设

描述物理体系的波函数对应于希尔伯特空间中的矢量，简称为态矢量。

对理论物理学家或数学家来说，

量子物理发生在希尔伯特空间。

然而我们需要牢记，

物理现象（经典或量子）是发生在实验室内。

狄拉克符号

为了将态矢量从具体坐标表示中释放出来，狄拉克引入符号

Ket矢 (右矢) $\psi \to |\psi\rangle$

Hilbert空间 $\mathcal{H}$

Bra矢 (左矢) $\psi^* \to \langle\psi|$

Hilbert空间的对偶空间 $\mathcal{H}_d = \mathcal{H}^*$

每一个右矢都存在一个单独的左矢，反之亦然。

内积： $(\phi, \psi) \to \langle\phi|\psi\rangle$

如果要研究粒子出现在空间某处（或某个动量）的概率，
我们需要写出粒子在坐标空间（或动量空间）中的波函数，

$$\psi(\vec{r}, t) = \langle\vec{r}, t|\psi\rangle \qquad \varphi(\vec{p}, t) = \langle\vec{p}, t|\psi\rangle$$

内积为 $\langle\phi|\psi\rangle = \int \phi^*(\vec{r}, t)\psi(\vec{r}, t)d^3r$

左矢和右矢的属性

每一个ket矢都有一个相应的bra矢

$$|\psi\rangle^* = \langle\psi| \qquad (\alpha\,|\psi\rangle)^* = \alpha^*\,\langle\psi|$$

$$|\alpha\psi\rangle = \alpha\,|\psi\rangle \qquad \langle\alpha\psi| = \alpha^*\,\langle\psi|$$

标积性质

$$\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$$

QM中标积为复数，顺序非常重要

$$\langle\psi|a_1\psi_1 + a_2\psi_2\rangle = a_1\,\langle\psi|\psi_1\rangle + a_2\,\langle\psi|\psi_2\rangle$$

线性

$$\langle a_1\psi_1 + a_2\psi_2|\psi\rangle = a_1^*\,\langle\psi_1|\psi\rangle + a_2^*\,\langle\psi_2|\psi\rangle$$

反线性

$$\begin{aligned}\langle a_1\phi_1 + a_2\phi_2|b_1\psi_1 + b_2\psi_2\rangle &= a_1^* b_1\,\langle\phi_1|\psi_1\rangle + a_1^* b_2\,\langle\phi_1|\psi_2\rangle \\ &\quad + a_2^* b_1\,\langle\phi_2|\psi_1\rangle + a_2^* b_2\,\langle\phi_2|\psi_2\rangle\end{aligned}$$

左矢和右矢的属性

标积满足Schwarz不等式

$$|\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle$$

标积满足三角不等式

$$\sqrt{\langle\psi+\phi|\psi+\phi\rangle} \leq \sqrt{\langle\psi|\psi\rangle} + \sqrt{\langle\phi|\phi\rangle} \qquad |\vec{A}+\vec{B}| \leq |\vec{A}| + |\vec{B}|$$

正交归一态

$$\langle\psi|\phi\rangle = 0 \qquad \langle\psi|\psi\rangle = 1 \qquad \langle\phi|\phi\rangle = 1$$

禁止的物理量

如果 $|\psi\rangle$ 和 $|\phi\rangle$ 属于同一希尔伯特空间，

$|\psi\rangle\,|\phi\rangle$ 和 $\langle\psi|\,\langle\phi|$ 是禁止的。属于不同空间可以直乘。

狄拉克符号总结

Dirac formalism	Wave functions
$\|\varphi\rangle$	$\varphi(\boldsymbol{r})$
$\|\psi(t)\rangle$	$\psi(\boldsymbol{r}, t)$
$\langle\psi_2\|\psi_1\rangle$	$\int \psi_2^*(\boldsymbol{r})\psi_1(\boldsymbol{r})\, d^3r$
$\\|\psi\\|^2 = \langle\psi\|\psi\rangle$	$\int \|\psi(\boldsymbol{r})\|^2\, d^3r$
$\langle\psi_2\|\hat{A}\|\psi_1\rangle$	$\int \psi_2^*(\boldsymbol{r})\hat{A}\psi_1(\boldsymbol{r})\, d^3r$
$\langle a\rangle = \langle\psi\|\hat{A}\|\psi\rangle$	$\int \psi^*(\boldsymbol{r})\hat{A}\psi(\boldsymbol{r})\, d^3r$

选定正交归一完备的Hilbert基

$$\{|n\rangle\}$$

$$\langle n|m\rangle = \delta_{nm}$$

任意矢量都可以展开为

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

$$C_n = \langle n|\psi\rangle$$

算 符

作用在态矢量上将之变换为另外一个态矢量

$$|\psi\rangle \xrightarrow{\hat{O}} |\phi\rangle$$

物理量：线性+厄米算符

$$\hat{A} = \hat{A}^\dagger$$

算符的厄米共轭是该算符取复共轭，再转置

$$\Big\langle \psi_2 | \hat{A} | \psi_1 \Big\rangle = \Big\langle \psi_2 | \hat{A}^\dagger | \psi_1 \Big\rangle = \Big\langle \psi_1 | \hat{A} | \psi_2 \Big\rangle^*$$

$$(\psi_2, \hat{A}\psi_1) = (\psi_2, \hat{A}^\dagger \psi_1) = (\psi_1, \hat{A}\psi_2)^*$$

$$\Rightarrow \quad \Big\langle \psi | \hat{A} | \psi \Big\rangle = \Big\langle \psi | \hat{A} | \psi \Big\rangle^*$$

厄米算符的平均值是实数

狄拉克符号法则

1） 左右矢缩并

特殊的线性算符 $|u\rangle\langle v|$

$$(|u\rangle\langle v|)|\psi\rangle = |u\rangle\langle v|\psi\rangle = \lambda|u\rangle$$

左矢$\langle v|$ “吃掉” 右矢$|\psi\rangle$，并给出复数$\lambda = \langle v|\psi\rangle$

2） 厄米共轭操作

如同有限维矩阵一样，我们先转置再取复共轭

1） 颠倒每一项顺序

2） $|u\rangle \leftrightarrow \langle u|$

3） $\hat{A} \rightarrow \hat{A}^\dagger$

4） 复数取复共轭

$$\lambda|\varphi\rangle\langle\psi|\hat{A}^\dagger\hat{B}$$

↕ 取厄米共轭

$$\lambda^*\hat{B}^\dagger\hat{A}|\psi\rangle\langle\varphi|$$

希尔伯特空间的张量积

两体系统的希尔伯特空间

$$\psi(\vec{r}_1,\vec{r}_2)=\phi(\vec{r}_1)\chi(\vec{r}_2)$$

第1个粒子 Hilbert空间$\mathcal{H}_1$ 的矢量

$$|\psi\rangle=|\phi\rangle\otimes|\chi\rangle$$

第2个粒子 Hilbert空间 $\mathcal{H}_2$ 的矢量

表明：第1个粒子处于$|\phi\rangle$　第2个粒子处于 $|\chi\rangle$

(1) 如果 $|n\rangle_1$ 和 $|m\rangle_2$ 分别是希尔伯特空间 $\mathcal{H}_1$ 和 $\mathcal{H}_2$ 的基矢，那么乘积

$$|n\rangle_1\otimes|m\rangle_2,\quad n,m=1,2,3,\cdots$$

形成两粒子希尔伯特空间的正交基矢。

$$\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2.$$

(2) 态矢量的乘积满足如下内积关系：

$$\Big(\langle\phi'|\otimes\langle\chi'|\Big)\Big(|\phi\rangle\otimes|\chi\rangle\Big)=\langle\phi'|\phi\rangle\langle\chi'|\chi\rangle$$

向量空间的扩充

直和 (direct sum) V(n): $\{\vec{e}_1, \vec{e}_2, \cdots, \vec{e}_n\}$

W(m): $\{\vec{f}_1, \vec{f}_2, \cdots, \vec{f}_m\}$

V+W (n+m): $\{\vec{e}_1, \cdots, \vec{e}_n, \vec{f}_1, \cdots, \vec{f}_m\}$

$$\vec{v} = \left.\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}_V \right\} n$$

$$\vec{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_V, \quad \vec{e}_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}_V, \quad \cdots, \quad \vec{e}_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}_V$$

$$\vec{v} = \underbrace{\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}_V}_{n} \qquad \vec{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_V, \quad \vec{e}_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}_V, \quad \cdots, \quad \vec{e}_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}_V$$

$$\vec{w} = \underbrace{\begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix}_W}_{m} \qquad \vec{f}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_W, \quad \vec{f}_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}_W, \quad \cdots, \quad \vec{f}_m = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}_W$$

$$\vec{v} \oplus \vec{w} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \\ \hline w_1 \\ \vdots \\ w_m \end{pmatrix} = \left.\begin{pmatrix} \vec{v} \\ \hline \vec{w} \end{pmatrix}\right\} n + m$$

矩阵 $\vec{v} \mapsto A\vec{v}$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}_V, \qquad B = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}_W$$

$$A \oplus B = \left(\begin{array}{c|c} A & 0_{n\times m} \\ \hline 0_{m\times n} & B \end{array}\right)$$

$$(A \oplus B)(\vec{v} \oplus \vec{w}) = \left(\begin{array}{c|c} A & 0_{n\times m} \\ \hline 0_{m\times n} & B \end{array}\right) \left(\begin{array}{c} \vec{v} \\ \hline \vec{w} \end{array}\right) = \left(\begin{array}{c} A\vec{v} \\ \hline B\vec{w} \end{array}\right) = (A\vec{v}) \oplus (B\vec{w})$$

$$(A_1 \oplus B_1)(A_2 \oplus B_2) = (A_1 A_2) \oplus (B_1 B_2)$$

向量空间的张量积

直乘 (direct product) VxW (*n* x *m*): $\vec{e}_i \otimes \vec{f}_j$

双线性

$$\vec{v} \otimes \vec{w} = (\sum_i^n v_i \vec{e}_i) \otimes (\sum_j^m w_j \vec{f}_j) = \sum_i^n \sum_j^m v_i w_j (\vec{e}_i \otimes \vec{f}_j)$$

V(2) 和 W(3)

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad \vec{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}.$$

$$\vec{e}_1 \otimes \vec{f}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \hline 0 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{e}_1 \otimes \vec{f}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \hline 0 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{e}_1 \otimes \vec{f}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \hline 0 \\ 0 \\ 0 \end{pmatrix},$$

$$\vec{e}_2 \otimes \vec{f}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \hline 1 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{e}_2 \otimes \vec{f}_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \hline 0 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{e}_2 \otimes \vec{f}_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \hline 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\vec{v} \otimes \vec{w} = \begin{pmatrix} v_1 w_1 \\ v_1 w_2 \\ v_1 w_3 \\ — \\ v_2 w_1 \\ v_2 w_2 \\ v_2 w_3 \end{pmatrix}.$$

矩阵

张量积空间中，矩阵A作用在矢量v上，同时不改变W

$$A_{2\times2}=\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix},\quad \hat{I}_{3\times3}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$A\otimes I=\left(\begin{array}{ccc|ccc} a_{11} & 0 & 0 & a_{12} & 0 & 0 \\ 0 & a_{11} & 0 & 0 & a_{12} & 0 \\ 0 & 0 & a_{11} & 0 & 0 & a_{12} \\ \hline a_{21} & 0 & 0 & a_{22} & 0 & 0 \\ 0 & a_{21} & 0 & 0 & a_{22} & 0 \\ 0 & 0 & a_{21} & 0 & 0 & a_{22} \end{array}\right)$$

矩阵作用在向量上

$$A\otimes I=\left(\begin{array}{ccc|ccc} a_{11} & 0 & 0 & a_{12} & 0 & 0\\ 0 & a_{11} & 0 & 0 & a_{12} & 0\\ 0 & 0 & a_{11} & 0 & 0 & a_{12}\\ \hline a_{21} & 0 & 0 & a_{22} & 0 & 0\\ 0 & a_{21} & 0 & 0 & a_{22} & 0\\ 0 & 0 & a_{21} & 0 & 0 & a_{22} \end{array}\right) \qquad \vec{v}\otimes\vec{w}=\begin{pmatrix} v_1w_1\\ v_1w_2\\ v_1w_3\\ \text{—}\\ v_2w_1\\ v_2w_2\\ v_2w_3 \end{pmatrix}$$

$$(A\otimes I)(\vec{v}\otimes\vec{w}) = \left(\begin{array}{ccc|ccc} a_{11} & 0 & 0 & a_{12} & 0 & 0\\ 0 & a_{11} & 0 & 0 & a_{12} & 0\\ 0 & 0 & a_{11} & 0 & 0 & a_{12}\\ \hline a_{21} & 0 & 0 & a_{22} & 0 & 0\\ 0 & a_{21} & 0 & 0 & a_{22} & 0\\ 0 & 0 & a_{21} & 0 & 0 & a_{22} \end{array}\right)\left(\begin{array}{c} v_1w_1\\ v_1w_2\\ v_1w_3\\ \hline v_2w_1\\ v_2w_2\\ v_2w_3 \end{array}\right) = \left(\begin{array}{c} (a_{11}v_1+a_{12}v_2)w_1\\ (a_{11}v_1+a_{12}v_2)w_2\\ (a_{11}v_1+a_{12}v_2)w_3\\ \hline (a_{21}v_1+a_{22}v_2)w_1\\ (a_{21}v_1+a_{22}v_2)w_2\\ (a_{21}v_1+a_{22}v_2)w_3 \end{array}\right)$$

$$= \begin{pmatrix} a_{11}v_1+a_{12}v_2\\ a_{21}v_1+a_{22}v_2 \end{pmatrix}\otimes\begin{pmatrix} w_1\\ w_2\\ w_3 \end{pmatrix} = (A\vec{v})\otimes\vec{w}.$$

显然，A 仅仅作用在 $\vec{v}\in\mathcal{V}$，并不改变 $\vec{w}\in\mathcal{W}$。

$$B = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}_W \qquad I \otimes B = \left(\begin{array}{ccc|ccc} b_{11} & b_{12} & b_{13} & 0 & 0 & 0 \\ b_{21} & b_{22} & b_{23} & 0 & 0 & 0 \\ b_{31} & b_{32} & b_{33} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & b_{11} & b_{12} & b_{13} \\ 0 & 0 & 0 & b_{21} & b_{22} & b_{23} \\ 0 & 0 & 0 & b_{31} & b_{32} & b_{33} \end{array}\right)$$

$$\begin{aligned}
(I \otimes B)(\vec{v} \otimes \vec{w}) &= \left(\begin{array}{ccc|ccc} b_{11} & b_{12} & b_{13} & 0 & 0 & 0 \\ b_{21} & b_{22} & b_{23} & 0 & 0 & 0 \\ b_{31} & b_{32} & b_{33} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & b_{11} & b_{12} & b_{13} \\ 0 & 0 & 0 & b_{21} & b_{22} & b_{23} \\ 0 & 0 & 0 & b_{31} & b_{32} & b_{33} \end{array}\right) \left(\begin{array}{c} v_1 w_1 \\ v_1 w_2 \\ v_1 w_3 \\ \hline v_2 w_1 \\ v_2 w_2 \\ v_2 w_3 \end{array}\right) \\
&= \left(\begin{array}{c} v_1(b_{11}w_1 + b_{12}w_2 + b_{13}w_3) \\ v_1(b_{21}w_1 + b_{22}w_2 + b_{23}w_3) \\ v_1(b_{31}w_1 + b_{32}w_2 + b_{33}w_3) \\ \hline v_2(b_{11}w_1 + b_{12}w_2 + b_{13}w_3) \\ v_2(b_{21}w_1 + b_{22}w_2 + b_{23}w_3) \\ v_2(b_{31}w_1 + b_{32}w_2 + b_{33}w_3) \end{array}\right) = \vec{v} \otimes (B\vec{w}).
\end{aligned}$$

$$A \otimes B = \left(\begin{array}{ccc|ccc} a_{11}b_{11} & a_{11}b_{12} & a_{11}b_{13} & a_{12}b_{11} & a_{12}b_{12} & a_{12}b_{13} \\ a_{11}b_{21} & a_{11}b_{22} & a_{11}b_{23} & a_{12}b_{21} & a_{12}b_{22} & a_{12}b_{23} \\ a_{11}b_{31} & a_{11}b_{32} & a_{11}b_{33} & a_{12}b_{31} & a_{12}b_{32} & a_{12}b_{33} \\ \hline a_{21}b_{11} & a_{21}b_{12} & a_{21}b_{13} & a_{22}b_{11} & a_{22}b_{12} & a_{22}b_{13} \\ a_{21}b_{21} & a_{21}b_{22} & a_{21}b_{23} & a_{22}b_{21} & a_{22}b_{22} & a_{22}b_{23} \\ a_{21}b_{31} & a_{21}b_{32} & a_{21}b_{33} & a_{22}b_{31} & a_{22}b_{32} & a_{22}b_{33} \end{array}\right)$$

$$(A \otimes B)(\vec{v} \otimes \vec{w}) = (A\vec{v}) \otimes (B\vec{w})$$

$$\begin{aligned} &(A_1 \otimes I)(A_2 \otimes I) = (A_1 A_2) \otimes I, \\ &(I \otimes B_1)(I \otimes B_2) = I \otimes (B_1 B_2), \\ &(A \otimes I)(I \otimes B) = (I \otimes B)(A \otimes I) = (A \otimes B) \end{aligned}$$

希尔伯特空间直乘

当量子系统存在两个或多个独立自由度时，希尔伯特空间都存在张量积。一个给定的希尔伯特空间可以有多种分解方法。 $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$

多种分解形式。例如，两体波函数 $\psi(\vec{r}_1, \vec{r}_2)$ 也可以写作为质心和相对运动坐标的函数。令

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}, \qquad \vec{r} = \vec{r}_1 - \vec{r}_2. \tag{A.1.6}$$

显然，$\psi(\vec{r}_1, \vec{r}_2)$ 的函数空间可以被 $\phi'(\vec{R})\chi'(\vec{r})$ 函数乘积所涵盖，因此有

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_{cm} \otimes \mathcal{H}_{rel}, \tag{A.1.7}$$

其中 $\mathcal{H}_{cm}$ 和 $\mathcal{H}_{rel}$ 分别表示质心坐标 $\vec{R}$ 和相对坐标 $\vec{r}$ 的函数空间。在处理中心势场问题时，$\mathcal{H}_{cm} \otimes \mathcal{H}_{rel}$ 更具有优势。

与波函数类似，算符也具有类似的乘积形式。如果 $\hat{A}$ 和 $\hat{B}$ 是分别作用在 $\mathcal{H}_1$ 和 $\mathcal{H}_2$ 上的算符，我们可以定义作用在 $\mathcal{H}$ 上的算符乘积 $\hat{A}\otimes\hat{B}$ 如下：

$$\left(\hat{A}\otimes\hat{B}\right)\left(\left|\phi\right\rangle\otimes|\chi\rangle\right)=\hat{A}\left|\phi\right\rangle\otimes\hat{B}|\chi\rangle. \tag{A.1.8}$$

两粒子体系的基本动力学变量都是 $\hat{A}\otimes\hat{I}$ 或 $\hat{I}\otimes\hat{B}$ 的形式。例如，第一个粒子的动量算符为

$$\hat{P}_1(\text{on }\mathcal{H})=\hat{P}_1(\text{on }\mathcal{H}_1)\otimes\hat{I}(\text{on }\mathcal{H}_2). \tag{A.1.9}$$

这意味着，当 $\hat{P}_1$ 作用在两粒子态矢量 $\left|\phi\right\rangle\otimes|\chi\rangle$ 上时，$\hat{P}_1$ 算符将 $\left|\phi\right\rangle$ 替换成 $\hat{P}_1\left|\phi\right\rangle$，但不改变 $|\chi\rangle$。当考虑两粒子体系空间波函数 $\psi(\vec{r}_1,\vec{r}_2)$ 时，上面算符乘积的定义意味着

$$\hat{P}_1=-i\hbar\nabla_1. \tag{A.1.10}$$

同理可得，第二个粒子的动量算符是

$$\hat{P}_2(\text{on }\mathcal{H})=\hat{I}_1(\text{on }\mathcal{H}_1)\otimes\hat{P}_2(\text{on }\mathcal{H}_2). \tag{A.1.11}$$

三维自由粒子

$$\left|p_x, p_y, p_z\right\rangle = |p_x\rangle \otimes \left|p_y\right\rangle \otimes |p_z\rangle$$

$$\hat{P}_x \ \rightarrow \ \hat{P}_x \otimes \hat{I}_y \otimes \hat{I}_z.$$

$$\begin{aligned}\left(\hat{P}_x \otimes \hat{I}_y \otimes \hat{I}_z\right)\left(|p_x\rangle \otimes \left|p_y\right\rangle \otimes |p_z\rangle\right) &= \left(\hat{P}_x \otimes |p_x\rangle\right) \otimes \left(\hat{I}_y \otimes \left|p_y\right\rangle\right) \otimes \left(\hat{I}_z \otimes |p_z\rangle\right) \\ &= p_x |p_x\rangle \otimes \left|p_y\right\rangle \otimes |p_z\rangle.\end{aligned}$$

三维自由粒子的哈密顿算符的完整形式是

$$\hat{H} = \frac{1}{2m}\left[\left(\hat{P}_x \otimes \hat{I}_y \otimes \hat{I}_z\right)^2 + \left(\hat{I}_x \otimes \hat{P}_y \otimes \hat{I}_z\right)^2 + \left(\hat{I}_x \otimes \hat{I}_y \otimes \hat{P}_z\right)^2\right]$$

2. 态矢量、表象和表示

态矢量、表象和表示

波函数可以抽象为希尔伯特空间中的一个态矢量 $|\psi\rangle$

力学量完全集 $\{\hat{F},\cdots\}$

共同本征函数组 $\{\phi_k\}$
正交完备归一的基矢 $\langle\phi_j|\phi_k\rangle=\delta_{jk}$

F表象

$$\forall\,|\psi\rangle,\ \ |\psi\rangle=\sum_k a_k\,|\phi_k\rangle\,,\ \ a_k=\langle\phi_k|\psi\rangle$$

F表象中坐标

选定一组力学量完全集(即选取坐标系)后, $\{a_k\}\equiv|\psi\rangle$

$\{a_k\}$：态矢量$|\psi\rangle$在F表象的表示

不同表象的表示仅仅是不同坐标系中对同一态矢量的描述。

投影算符

任意态矢量 $|\psi\rangle$在F表象中的表示

$$|\psi\rangle = \sum_k a_k |\phi_k\rangle = \sum_k \langle\phi_k|\psi\rangle |\phi_k\rangle = \sum_k \underbrace{|\phi_k\rangle\langle\phi_k|}_{\hat{\mathbb{P}}_k}\psi\rangle$$

$$\hat{\mathbb{P}}_k \equiv |\phi_k\rangle\langle\phi_k|$$

将态矢量 $|\psi\rangle$投影到第$|\phi_k\rangle$ 个基矢方向

$|\psi\rangle$是任意并且厄米算符的本征函数是完备的

→ 封闭性

$$\sum_k |\phi_k\rangle\langle\phi_k| = \hat{\mathbb{I}} \quad 离散谱$$

$$\int |\alpha\rangle d\alpha \langle\alpha| = \hat{\mathbb{I}} \quad 连续谱$$

投影算符示例

二维平面上矢量 $\vec{R} = a\vec{e}_x + b\vec{e}_y$

$$\vec{R} = \begin{pmatrix} a \\ b \end{pmatrix} \qquad \vec{e}_x = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \vec{e}_y = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{\mathbb{P}}_x = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{\mathbb{P}}_y = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\mathbb{P}}_x \vec{R} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a\vec{e}_x,$$

$$\hat{\mathbb{P}}_y \vec{R} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = b \begin{pmatrix} 0 \\ 1 \end{pmatrix} = b\vec{e}_y.$$

坐标表象

本征方程 $\hat{x}\left|x\right\rangle = x\left|x\right\rangle, \quad \forall x \in \mathbb{R}$

正交归一 $\langle x | x' \rangle = \delta(x - x')$

封闭性 $\int_{-\infty}^{+\infty} \left|x\right\rangle dx \left\langle x\right| = \mathbb{I}$

波函数归一化

$$\langle \psi | \psi \rangle = \langle \psi | \left(\int |x\rangle dx \langle x| \right) |\psi\rangle = \int \langle \psi | x \rangle \langle x | \psi \rangle dx$$

$$= \int \psi^*(x)\psi(x)dx = 1$$

↓

坐标空间
波函数

坐标表象

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \quad \rightarrow \quad \psi(x) = \sum_n c_n \phi_n(x)$$

$$\left(\int |x\rangle\, dx\, \langle x|\right) |\psi\rangle = \sum_n c_n \left(\int |x\rangle\, dx\, \langle x|\right) |\phi_n\rangle$$

$$\rightarrow \int dx\, |x\rangle\, \psi(x) = \sum_n c_n \int dx\, |x\rangle\, \phi_n(x)$$

将等式两方和$\langle x'|$做内积（假设积分和求和可以互换）

$$\int dx\, \langle x' |x\rangle\, \psi(x) = \sum_n c_n \int dx\, \langle x' |x\rangle\, \phi_n(x)$$

$$\int dx \delta(x' - x)\psi(x) = \sum_n c_n \int dx \delta(x' - x)\phi_n(x)$$

$$\rightarrow \quad \psi(x') = \sum_n c_n \phi_n(x')$$

表象变换

态矢量 $|\psi\rangle$ 在F表象 $\{|\phi_k\rangle\}$ 和 F'表象 $\{|\phi'_k\rangle\}$ 中的表示

$$|\psi\rangle = \sum_k a_k |\phi_k\rangle = \sum_\alpha a'_\alpha |\phi'_\alpha\rangle$$

$$\Rightarrow \langle\phi'_\beta|\psi\rangle = \sum_k a_k \langle\phi'_\beta|\phi_k\rangle = \sum_\alpha a'_\alpha \underbrace{\langle\phi'_\beta|\phi'_\alpha\rangle}_{\delta_{\alpha\beta}} = \sum_\alpha a'_\alpha \delta_{\alpha\beta} = a'_\beta$$

$$\Rightarrow a'_\beta = \sum_k a_k \langle\phi'_\beta|\phi_k\rangle \equiv \sum_k S_{\beta k} a_k$$ 其中 $S_{\beta k} \equiv \langle\phi'_\beta|\phi_k\rangle$

$$\begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle\phi'_1|\phi_1\rangle & \langle\phi'_1|\phi_2\rangle & \cdots \\ \langle\phi'_2|\phi_1\rangle & \langle\phi'_2|\phi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = \underbrace{\begin{pmatrix} S_{11} & S_{12} & \cdots \\ S_{21} & S_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}_{S_{F' \leftarrow F}} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

坐标表象和动量表象之间变换

本征方程	$\hat{x}\,\|x\rangle = x\,\|x\rangle$	$\hat{p}\,\|p\rangle = p\,\|p\rangle$
正交归一	$\langle x\,\|x'\rangle = \delta(x-x')$	$\langle p\,\|p'\rangle = \delta(p-p')$
封闭性	$\int \|x\rangle\, dx\, \langle x\| = \mathbb{I}$	$\int \|p\rangle\, dp\, \langle p\| = \mathbb{I}$

$$\psi(p) = \langle p\,|\psi\rangle = \int dx\,\langle p\,|x\rangle\,\langle x\,|\psi\rangle = \int dx\,\langle p\,|x\rangle\,\psi(x)$$

$$\psi(x) = \langle x\,|\psi\rangle = \int dp\,\langle x\,|p\rangle\,\langle p\,|\psi\rangle = \int dp\,\langle x\,|p\rangle\,\psi(p)$$

变换系数 $\langle x\,|p\rangle$ 和 $\langle p\,|x\rangle$ 是什么?

$$\langle x|p\rangle = ? \qquad \langle p|x\rangle = ?$$

① $\hat{P}|p\rangle = p|p\rangle \rightarrow \left\langle x\middle|\hat{P}\middle|p\right\rangle = p\langle x|p\rangle \rightarrow \int dx' \left\langle x\middle|\hat{P}\middle|x'\right\rangle \langle x'|p\rangle = p\langle x|p\rangle$

本征方程

② $i\hbar\langle x|x'\rangle = \left\langle x\middle|\hat{X}\hat{P}\middle|x'\right\rangle - \left\langle x\middle|\hat{P}\hat{X}\middle|x'\right\rangle = (x-x')\left\langle x\middle|\hat{P}\middle|x'\right\rangle \rightarrow \left\langle x\middle|\hat{P}\middle|x'\right\rangle = \frac{i\hbar\delta(x-x')}{(x-x')}$

对易关系

$$\rightarrow p\langle x|p\rangle = \int dx' i\hbar \frac{\delta(x-x')}{(x-x')}\langle x'|p\rangle$$

将 $\langle x'|\psi\rangle$ 在 $\langle x|\psi\rangle$ 附近展开

$$\langle x'|p\rangle = \langle x|p\rangle + (x'-x)\frac{d}{dx}\langle x|p\rangle + \frac{(x'-x)^2}{2}\frac{d^2}{dx^2}\langle x|p\rangle + \cdots$$

则有

$$-\frac{i}{\hbar}p\langle x|p\rangle = \int dx'\frac{\delta(x-x')}{(x-x')}\left[\langle x|p\rangle + (x'-x)\frac{d}{dx}\langle x|p\rangle + \frac{(x'-x)^2}{2}\frac{d^2}{dx^2}\langle x|p\rangle + \cdots\right]$$

$$= \langle x|p\rangle\int dx'\frac{\delta(x-x')}{(x-x')} - \frac{d}{dx}\langle x|p\rangle\underbrace{\int dx'\delta(x-x')}_{=1}$$

$$+\frac{d^2}{dx^2}\langle x|p\rangle\underbrace{\int dx'(x-x')\delta(x-x')}_{\rightarrow 0} + \underbrace{\{\quad\cdots\quad\}}_{\rightarrow 0}$$

$$\langle x\,|p\rangle = ? \qquad \langle p\,|x\rangle = ?$$

$$\int dx' \frac{\delta(x-x')}{(x-x')} = \lim_{\sigma\to 0} \frac{1}{\sqrt{\pi\sigma^2}} \int_{-\infty}^{+\infty} dx' \frac{e^{-(x-x')^2/\sigma^2}}{(x-x')}$$

$$= \lim_{\sigma\to 0} \frac{1}{\sqrt{\pi\sigma^2}} \int_{-\infty}^{+\infty} dx \frac{e^{-x^2/\sigma^2}}{x} \xrightarrow{\text{odd function}} 0$$

$$\frac{i}{\hbar} p \langle x\,|p\rangle = \frac{d}{dx} \langle x\,|p\rangle \rightarrow \int \frac{1}{\langle x\,|p\rangle} d\langle x\,|p\rangle = \int \frac{i}{\hbar} p dx \rightarrow \langle x\,|p\rangle = Ce^{i\frac{px}{\hbar}}$$

归一化因子C

$$\delta(x-x') = \langle x\,|x'\rangle = \int dp \langle x\,|p\rangle \langle p\,|x'\rangle = \int dp |C|^2 e^{i\frac{p(x-x')}{\hbar}}$$

$$= |C|^2 2\pi\delta\left(\frac{x-x'}{\hbar}\right) = |C|^2 2\pi\hbar\delta(x-x') \rightarrow C = \frac{1}{\sqrt{2\pi\hbar}}$$

$$\langle x\,|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad , \quad \langle p\,|x\rangle = \langle x\,|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

动量算符微分形式

考虑一般性态矢量$|\psi\rangle$

$$\left\langle x\middle|\hat{P}\middle|\psi\right\rangle = \int dx' \left\langle x\middle|\hat{P}\middle|x'\right\rangle \langle x' \, |\psi\rangle$$

将$\langle x' \, |\psi\rangle$ 在 $\langle x \, |\psi\rangle$ 附近展开

$$\langle x' \, |p\rangle = \langle x \, |p\rangle + (x'-x)\frac{d}{dx}\langle x \, |p\rangle + \frac{(x'-x)^2}{2}\frac{d^2}{dx^2}\langle x \, |p\rangle + \cdots$$

$$\left\langle x\middle|\hat{P}\middle|x'\right\rangle = \frac{i\hbar\delta(x-x')}{(x-x')}$$

仅有一阶导数项不为零，故而

$$\boxed{\left\langle x\middle|\hat{P}\middle|\psi\right\rangle = -i\hbar\frac{d}{dx}\langle x \, |\psi\rangle} \Longrightarrow \hat{P} = -i\hbar\frac{d}{dx}$$

$$\hat{P} = -i\hbar\int dx \, |x\rangle \frac{d}{dx}\langle x|$$

3. 算符的表示

算符的自然展开

考虑力学量算符 $\hat{L}$ 在某力学量算符 $\hat{A}$ 表象（基矢为 $|\alpha\rangle$）中的表示。利用厄米算符本征矢量的封闭性，$\sum_\alpha |\alpha\rangle\langle\alpha| = \hat{I}$，可得 $\hat{L}$ 算符在 $\hat{A}$ 表象的自然展开

$$\hat{L} = \sum_{\alpha,\beta} |\alpha\rangle\langle\alpha|\hat{L}\left|\beta\rangle\langle\beta\right| = \sum_{\alpha,\beta} |\alpha\rangle L_{\alpha\beta}\left\langle\beta\right|.$$

当 $\hat{A} = \hat{L}$ 时，$\left\langle\alpha\middle|\hat{L}\middle|\beta\right\rangle = L_\beta\delta_{\alpha\beta}$，所以我们得到了力学量算符 $\hat{L}$ 的自然展开形式

$$\hat{L} = \sum_{\alpha\beta} |L_\alpha\rangle L_{\alpha\beta}\left\langle L_\beta\right| = \sum_{\alpha} |L_\alpha\rangle L_\alpha \langle L_\alpha|,$$

或当 $\hat{L}$ 本征函数为连续谱时

$$\hat{L} = \int |L\rangle L \langle L| dL.$$

算符的函数和逆

算符的自然展开也可以用来定义算符的函数

$$F(\hat{A}) = \sum_m |A_m\rangle F(A_m) \langle A_m| = \sum_m |A_m\rangle \sum_n \frac{F^{(n)}(0)}{n!} (A_m)^n \langle A_m|$$

逆算符 $\hat{A}^{-1}$ 定义为：$\hat{A}^{-1} = \sum_n |A_n\rangle \frac{1}{A_n} \langle A_n|$

$$\hat{A}\hat{A}^{-1} = \hat{A} \sum_n |A_n\rangle \frac{1}{A_n} \langle A_n| = \sum_n \hat{A} |A_n\rangle \frac{1}{A_n} \langle A_n|$$

$$= \sum_n A_n |A_n\rangle \frac{1}{A_n} \langle A_n| = \sum_n |A_n\rangle \langle A_n| = \hat{I}$$

$$\hat{A}^{-1}\hat{A} = \sum_n |A_n\rangle \frac{1}{A_n} \langle A_n| \hat{A} = \sum_n |A_n\rangle \frac{1}{A_n} \langle A_n| A_n^*$$

$$= \sum_n |A_n\rangle \frac{1}{A_n} \langle A_n| A_n = \sum_n |A_n\rangle \langle A_n| = \hat{I}$$

算符的表示

算符的操作： $|\varphi\rangle = \hat{L}\left|\psi\right\rangle$

在F表象中： $|\varphi\rangle = \sum_k b_k |\phi_k\rangle$ ， $|\psi\rangle = \sum_k a_k |\phi_k\rangle$

$$\sum_k b_k |\phi_k\rangle = \sum_k a_k \hat{L} |\phi_k\rangle$$

$$\sum_k b_j \underbrace{\langle\phi_j|\phi_k\rangle}_{\delta_{jk}} = \sum_k a_k \underbrace{\langle\phi_j|\hat{L}|\phi_k\rangle}_{L_{jk}} \quad \Longrightarrow \quad b_j = \sum_k L_{jk} a_k$$

$$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix} = \underbrace{\begin{pmatrix} L_{11} & L_{12} & \cdots \\ L_{21} & L_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}_{\equiv [L_{jk}]} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

L算符在F表象中的表示

矩阵$[L_{jk}]$描述了F表象的本征基矢$|\phi_k\rangle$在算符 $\hat{L}$ 的作用下所得到的新态矢量$\hat{L}|\phi_k\rangle$在F表象中的表示

$$\hat{L}|\phi_k\rangle = \sum_j |\phi_j\rangle\langle\phi_j| \ \hat{L}|\phi_k\rangle = \sum_j |\phi_j\rangle \ \left\langle\phi_j\middle|\hat{L}\middle|\phi_k\right\rangle = \sum_j |\phi_j\rangle L_{jk}$$

即 $\hat{L}|\phi_k\rangle = |\phi_1\rangle L_{1k} + |\phi_2\rangle L_{2k} + |\phi_3\rangle L_{3k} + \cdots$

$\{L_{1k}, L_{2k}, L_{3k}, \cdots\}$ 组成 $\hat{L}$ 算符在 $\hat{F}$ 表象中矩阵表示的第 k 列元素集合

$$\hat{L}|\phi_1\rangle = |\phi_1\rangle L_{11} + |\phi_2\rangle L_{21} + |\phi_3\rangle L_{31} + \cdots$$

$$\hat{L}|\phi_2\rangle = |\phi_1\rangle L_{12} + |\phi_2\rangle L_{22} + |\phi_3\rangle L_{32} + \cdots$$

$$\hat{L}|\phi_3\rangle = |\phi_1\rangle L_{13} + |\phi_2\rangle L_{23} + |\phi_3\rangle L_{33} + \cdots$$

$$\begin{pmatrix} L_{11} & L_{21} & L_{31} & \cdots \\ L_{12} & L_{22} & L_{32} & \cdots \\ L_{13} & L_{23} & L_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \xrightarrow{\text{转置}} [\hat{L}]_F = \begin{pmatrix} L_{11} & L_{12} & L_{13} & \cdots \\ L_{21} & L_{22} & L_{23} & \cdots \\ L_{31} & L_{32} & L_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

算符在自身表象的表示

算符在自身表象中的表示是对角矩阵，
而矩阵元为其本征值。

设算符 $\hat{A}$ 的本征态矢量为$|\alpha_i\rangle$，满足

$$\hat{A}\,|\alpha_i\rangle = \alpha_i\,|\alpha_i\rangle$$

算符 $\hat{A}$ 在自身表象中矩阵表示是

$$[A] = \begin{pmatrix} \alpha_1 & 0 & 0 & \cdots \\ 0 & \alpha_2 & 0 & \cdots \\ 0 & 0 & \alpha_3 & \cdots \\ \cdots & \cdots & \cdots & \ddots \end{pmatrix}$$

例I）哈密顿算符

$$\hat{H} = \sum_i |E_i\rangle E_i \langle E_i|$$

在 $\hat{H}$ 表象（能量表象）中，哈密顿算符形式为

$$\hat{H} = \begin{pmatrix} E_1 & 0 & 0 & \cdots \\ 0 & E_2 & 0 & \cdots \\ 0 & 0 & E_3 & \cdots \\ 0 & 0 & 0 & \ddots \end{pmatrix}$$

例2）简谐振子势的坐标和动量算符

设简谐振子势的本征函数为 $\{\phi_n(x),\quad n=0,1,2,\cdots\}$

$$\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^\dagger\right),\quad \hat{p}=i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}^\dagger-\hat{a}\right)$$

$$\hat{x}\phi_n(x) = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\phi_{n+1}(x)+\sqrt{n}\,\phi_{n-1}(x)\right),$$

$$\hat{p}\phi_n(x) = i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{n}\,\phi_{n-1}(x)-\sqrt{n+1}\,\phi_{n+1}(x)\right)$$

$$\hat{x} \Longrightarrow \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad \hat{p} \Longrightarrow i\sqrt{\frac{m\hbar\omega}{2}}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\hat{x}_{nk}\hat{p}_{km}-\hat{p}_{nk}\hat{x}_{km}=\mathbf{I}_{nm}$$

无限维

算符的表象变换

F 表象 (基矢 $\{|\phi_k\rangle\}$)：$L_{kj}=\langle\phi_k|\hat{L}|\phi_j\rangle$ $\longrightarrow$ F' 表象 (基矢 $\{|\phi'_\alpha\rangle\}$)：$L'_{\alpha\beta}=\langle\phi'_\alpha|\hat{L}|\phi'_\beta\rangle$

$$|\phi'_\alpha\rangle=\sum_k|\phi_k\rangle\langle\phi_k|\phi'_\alpha\rangle=\sum_k|\phi_k\rangle S^*_{\alpha k}$$

$$|\phi'_\beta\rangle=\sum_j|\phi_j\rangle\langle\phi_j|\phi'_\beta\rangle=\sum_j S^*_{\beta j}|\phi_j\rangle$$

$$L'_{\alpha\beta}=\langle\phi'_\alpha|\hat{L}|\phi'_\beta\rangle=\left(\sum_k\langle\phi_k|S_{\alpha k}\right)\hat{L}\left(\sum_j S^*_{\beta j}|\phi_j\rangle\right)$$

$$=\sum_{kj}S_{\alpha k}S^*_{\beta j}\langle\phi_k|\hat{L}|\phi_j\rangle$$

$$=\sum_{kj}S_{\alpha k}L_{kj}S^\dagger_{j\beta}=\left(SLS^\dagger\right)_{\alpha\beta}$$

简记为 $L'=SLS^\dagger=SLS^{-1},\quad L'\equiv[L'_{\alpha\beta}],\ L=[L_{kj}]$

Theorem 6.1 态矢量和力学量表示小结

	F 表象 $\{\|\phi_k\rangle\}$	F' 表象 $\{\|\phi'_\alpha\rangle\}$
态矢 $\|\psi\rangle$	$a=\begin{pmatrix}a_1\\a_2\\\vdots\end{pmatrix},\ a_k=\langle\phi_k\|\psi\rangle$	$a'=\begin{pmatrix}a'_1\\a'_2\\\vdots\end{pmatrix},\ a'_\alpha=\langle\phi'_\alpha\|\psi\rangle$
算符 $\hat{L}$	$L=[L_{kj}]=\begin{pmatrix}L_{11}&L_{12}&\cdots\\L_{21}&L_{22}&\cdots\\\vdots&\vdots&\ddots\end{pmatrix}$	$L'=[L'_{\alpha\beta}]=\begin{pmatrix}L'_{11}&L'_{12}&\cdots\\L'_{21}&L'_{22}&\cdots\\\vdots&\vdots&\ddots\end{pmatrix}$
	$L_{kj}=\left\langle\phi_k\middle\|\hat{L}\middle\|\phi_j\right\rangle$	$L'_{\alpha\beta}=\left\langle\phi'_\alpha\middle\|\hat{L}\middle\|\phi'_\beta\right\rangle$
表象变换		
	$F\to F'$	$F'\to F$
	$a'=Sa$	$a=S^\dagger a'$
	$L'=SLS^\dagger=SLS^{-1}$	$L=S^\dagger L'S$

其中

$$S=[S_{\alpha k}]=\begin{pmatrix}S_{11}&S_{12}&\cdots\\S_{21}&S_{22}&\cdots\\\vdots&\vdots&\ddots\end{pmatrix},\quad S_{\alpha k}=\left\langle\phi'_\beta\middle|\phi_k\right\rangle$$

4. 量子力学的矩阵形式

1）本征方程
2）定态薛定谔方程
3）平均值

I）本征方程

$$\hat{L}\left|\psi\right\rangle = L'\left|\psi\right\rangle \qquad \left|\psi\right\rangle = \sum_k a_k \left|\phi_k\right\rangle$$

$$\hat{L}\sum_k a_k\left|\phi_k\right\rangle = \sum_k a_k \hat{L}\left|\phi_k\right\rangle = L'\sum_k a_k\left|\phi_k\right\rangle$$

$$\sum_k a_k \underbrace{\left\langle\phi_j\middle|\hat{L}\middle|\phi_k\right\rangle}_{L_{jk}} = L'\sum_k a_k\left\langle\phi_j\middle|\phi_k\right\rangle = L'\sum_k a_k\delta_{jk} = L' a_j$$

$$\longrightarrow \sum_k \left(L_{jk} - L'\delta_{jk}\right) a_k = 0$$

存在非平庸解:

$$\det\left|L_{jk}-L'\delta_{jk}\right|=\begin{vmatrix} L_{11}-L' & L_{12} & L_{13} & \cdots \\ L_{21} & L_{22}-L' & L_{23} & \cdots \\ L_{31} & L_{32} & L_{33}-L' & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix}=0$$

求解出L本征值L'后，代入到本征方程中可得本征矢量

在 F 表象中和 L'_j 相应的本征矢量 a_k^j

$$\begin{pmatrix} a_1^{(j)} \\ a_2^{(j)} \\ \vdots \end{pmatrix}, \quad j=1,2,\cdots,N.$$

假设此本征方程组的维度为N

例1：泡利矩阵$\hat{\sigma}_x$在$\hat{\sigma}_z$表象中的本征值和本征矢

在σ_z表象 $\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

其本征方程的行列式如下：

$$\begin{vmatrix} -L' & 1 \\ 1 & -L' \end{vmatrix} = 0 \quad \Longrightarrow \quad L' = \pm 1$$

设待求解的本征矢为 $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$

$L' = +1$ → $\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0 \quad \Longrightarrow \quad a_1 = a_2$

$L' = -1$ → $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0 \quad \Longrightarrow \quad a_1 = -a_2$

在 σ_z 表象中 $\hat{\sigma}_x$ 的本征值和本征矢如下：

$$L' = +1 \quad : \quad |\sigma_x = +1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$L' = -1 \quad : \quad |\sigma_x = -1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

σ_x 表象到 σ_z 表象的变换矩阵

$$S_{\sigma_z \sigma_x} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$[\sigma_x]_{\text{自身表象}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\begin{aligned} [\sigma_x]_{\sigma_z\text{表象}} &= S\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}S^\dagger \\ &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

2）在 $\sigma_z=+1$ 的本征态中测量 $\hat{\sigma}_x$ 的可能值的概率？

$$A_{\sigma_x=+1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}},$$

$$A_{\sigma_x=-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}.$$

$$|\sigma_z=+1\rangle = \frac{1}{\sqrt{2}}|\sigma_x=+1\rangle + \frac{1}{\sqrt{2}}|\sigma_x=-1\rangle$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\times\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{\sqrt{2}}\times\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\Rightarrow \begin{cases} \sigma_x=+1 & : \quad \text{Prob} = \dfrac{1}{2}, \\ \sigma_x=-1 & : \quad \text{Prob} = \dfrac{1}{2}. \end{cases}$$

例2： 在$\{L^2, L_z\}$表象中， 求在$l=1$子空间中$\hat{L}_x$的本征值和本征矢

$$\hat{L}_+|lm\rangle = \hbar\sqrt{(l-m)(l+m+1)}\,|l,m+1\rangle$$

$$\hat{L}_-|lm\rangle = \hbar\sqrt{(l+m)(l-m+1)}\,|l,m-1\rangle$$

$$\begin{aligned}\hat{L}_x|lm\rangle &= \frac{\hat{L}_+ + \hat{L}_-}{2}|lm\rangle \\ &= \frac{\hbar}{2}\sqrt{(l+m)(l-m+1)}\,|l,m-1\rangle \\ &+ \frac{\hbar}{2}\sqrt{(l-m)(l+m+1)}\,|l,m+1\rangle\end{aligned}$$

$$\Rightarrow \quad [L_x] = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$\hat{L}_x\,|1,-1\rangle$ $\hat{L}_x\,|1,0\rangle$ $\hat{L}_x\,|1,1\rangle$

其本征方程

$$\sum_n \left[\left(\hat{L}_x \right)_{mn} - l_x \hbar \delta_{mn} \right] a_n = 0,$$

$$\begin{pmatrix} -l_x & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & -l_x & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & -l_x \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \qquad \begin{vmatrix} -l_x & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & -l_x & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & -l_x \end{vmatrix} = 0 \quad \Rightarrow \quad -l_x^3 + l_x = 0$$

本征值和本征矢

$$l_x = 1 \qquad\qquad l_x = 0 \qquad\qquad l_x = 1$$

$$\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \qquad \frac{1}{2}\begin{pmatrix} \sqrt{2} \\ 0 \\ -\sqrt{2} \end{pmatrix} \qquad \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}.$$

求在 $\hat{L}_z$ 的本征值为 0 的本征态中测量 $\hat{L}_x$ 的可取值的概率？

$$|L=1,L_z=0\rangle=\begin{pmatrix}0\\1\\0\end{pmatrix}=\frac{\sqrt{2}}{2}\times\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}-\frac{\sqrt{2}}{2}\times\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}$$

$$A_{+\hbar}=\frac{1}{2}\begin{pmatrix}1 & \sqrt{2} & 1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}=\frac{\sqrt{2}}{2},\qquad A_0=\frac{1}{2}\begin{pmatrix}\sqrt{2} & 0 & -\sqrt{2}\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}=0$$

$$A_{-\hbar}=\frac{1}{2}\begin{pmatrix}1 & -\sqrt{2} & 1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}=-\frac{\sqrt{2}}{2}$$

在 L_z 表象中本征值为$l_z=0$ 的本征矢中测量 $\hat{L}_x$ 的可能值和相应的概率

$$\begin{aligned}L_x=+\hbar &\quad:\quad \mathrm{Prob}=\frac{1}{2},\\ L_x=0 &\quad:\quad 0\quad ,\\ L_x=-\hbar &\quad:\quad \mathrm{Prob}=\frac{1}{2}.\end{aligned}$$

通过表象变换给出 $\hat{L}_x$ 在 $\{L^2, L_x\}$ 表象中的矩阵形式

$\{L^2, L_x\}$ 到 $\{L^2, L_z\}$ 表象的变换矩阵是

$$S_{L_z L_x} = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix},$$

从 $\{L^2, L_z\}$ 到 $\{L^2, L_x\}$ 表象的变换矩阵是

$$S_{L_x L_z} = S^\dagger_{L_z L_x} = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}$$

故而，$\hat{L}_x$ 在 $\{L^2, L_x\}$ 表象中的矩阵表示为

$$
\begin{aligned}
[L_x]_{L_x\text{表象}} &= S'\,[L_x]_{L_z\text{表象}}\,S'^{\dagger} = S^{\dagger}\,[L_x]_{L_z\text{表象}}\,S \\
&= \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \\
&= \frac{\hbar}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & -1 \\ \sqrt{2} & 0 & \sqrt{2} \\ 1 & 0 & -1 \end{pmatrix} \\
&= \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}
\end{aligned}
$$

2）定态薛定谔方程

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle$$

在F表象中

$$\left|\psi(t)\right\rangle = \sum_k a_k(t)\left|\phi_k\right\rangle$$

$$i\hbar\sum_k \frac{da_k}{dt}\left|\phi_k\right\rangle = \sum_k a_k(t)\hat{H}\left|\phi_k\right\rangle \rightarrow i\hbar\sum_k \frac{da_k}{dt}\underbrace{\left\langle\phi_j\middle|\phi_k\right\rangle}_{\delta_{jk}} = \sum_k a_k\left\langle\phi_j\middle|\hat{H}\middle|\phi_k\right\rangle$$

$$\Longrightarrow \quad i\hbar\frac{da_j}{dt} = \sum_k H_{jk}a_k.$$

$$i\hbar\frac{d}{dt}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & H_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$$i\hbar\frac{d}{dt}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & H_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

当F表象是哈密顿算符表象时,

$$H_{jk} = E_j \delta_{jk}$$

$$i\hbar\frac{da_j(t)}{dt} = E_j a_j(t) \quad \Longrightarrow \quad a_j(t) = a_j^0 e^{-i\hbar\frac{E_1 t}{\hbar}}, \;\; a_j^0 \equiv a_j(t=0)$$

在H表象中,
薛定谔方程是
对角化的

$$\left|\psi(t)\right\rangle = \begin{pmatrix} a_1^0 e^{-i\frac{E_1 t}{\hbar}} \\ a_2^0 e^{-i\frac{E_2 t}{\hbar}} \\ \vdots \end{pmatrix}$$

3）平均值

在 F 表象中，力学量算符 $\hat{L}$ 在态矢量 $|\psi\rangle$ 中的平均值为

$$\langle L\rangle=\langle\psi|\hat{L}|\psi\rangle=\sum_{jk}a_j^*\langle\phi_j|\hat{L}|\phi_k\rangle a_k=\sum_{jk}a_j^*a_kL_{jk},$$

矩阵形式是

$$\langle L\rangle=\begin{pmatrix}a_1^* & a_2^* & \cdots\end{pmatrix}\begin{pmatrix}L_{11} & L_{12} & \cdots\\ L_{21} & L_{22} & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}a_1\\ a_2\\ \vdots\end{pmatrix}.$$

如果我们选取 $\hat{L}$ 表象，即用 $\hat{L}$ 本征矢作为基矢，那么 $[L_{jk}]$ 就是一个对角矩阵
$\hat{L}$ 的平均值是

$$\langle L\rangle=\sum_{jk}a_j^*\langle\phi_j|\hat{L}|\phi_k\rangle a_k=\sum_{jk}a_j^*L_j\delta_{jk}a_k=\sum_{k}|a_k|^2L_k$$

5. 薛定谔绘景和海森堡绘景

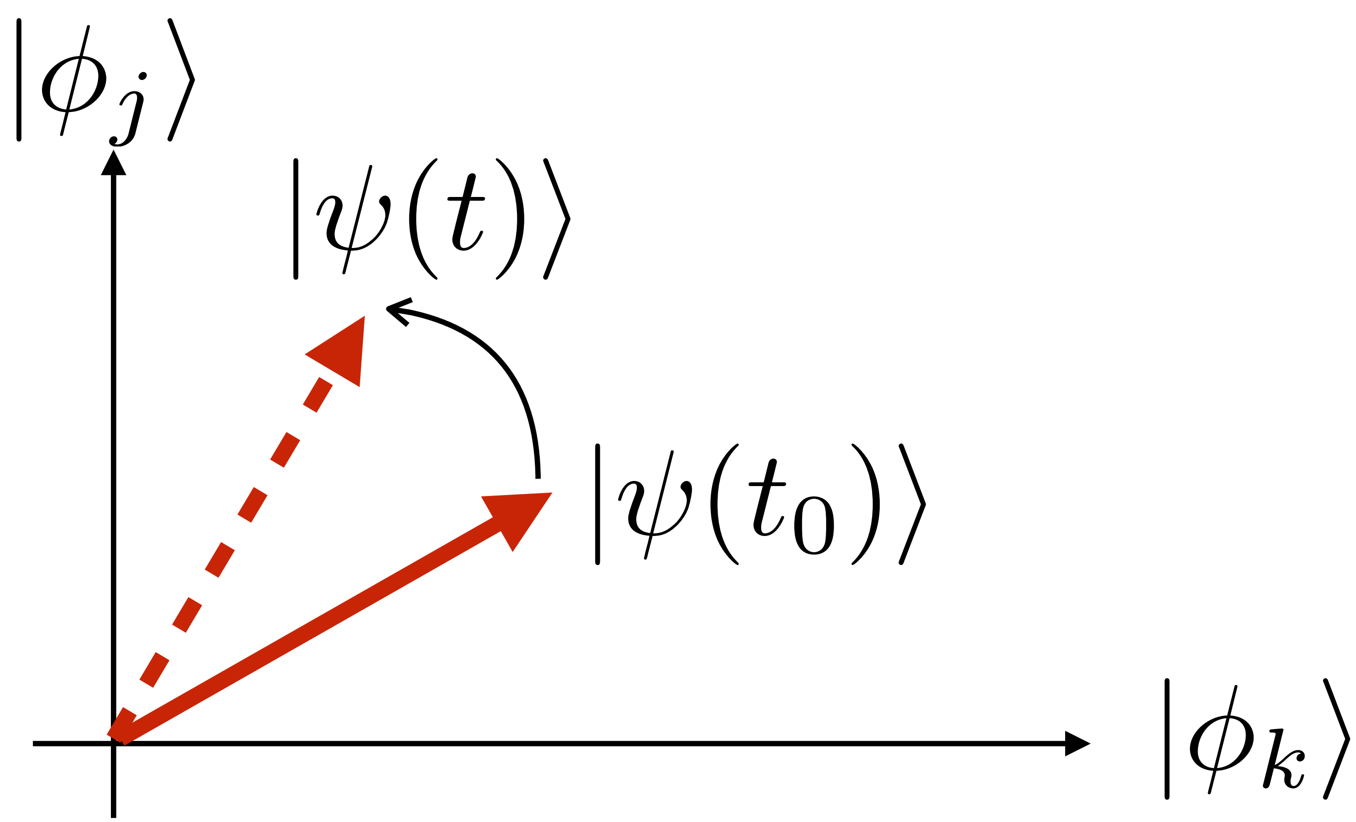
1）时间演化算符

2）海森堡方程

薛定谔绘景

在薛定谔波动力学中，力学量算符不显含时间，其平均值及其几率分布随时间演化完全归于态矢量$|\psi\rangle$随时间的演化

$$\frac{d}{dt}\langle F\rangle = \frac{1}{i\hbar}\overline{[\hat{F},\hat{H}]}$$



问：是否还有其他等效的描述?

时间演化算符

设波函数随时间演化的行为由时间演化算符$\hat{U}(t,t_i)$描述

设 $t_i = 0$ $$|\psi(t)\rangle = \hat{U}(t,0)\,|\psi(0)\rangle\,,\quad \hat{U}(0,0)=1$$

态叠加原理要求$\hat{U}(t,0)$ 是线性算符

$$\hat{U}(t,0)(a\,|\psi_1(0)\rangle + b\,|\psi_2(0)\rangle) = a\hat{U}(t,0)\,|\psi_1(0)\rangle + b\hat{U}(t,0)\,|\psi_2(0)\rangle$$

几率守恒要求 $\langle\psi(t)\,|\psi(t)\rangle = \langle\psi(0)\,|\psi(0)\rangle$

$$\begin{aligned}\langle\psi(t)\,|\psi(t)\rangle &= \left\langle\hat{U}(t,0)\psi(0)\,\middle|\hat{U}(t,0)\psi(0)\right\rangle\\ &= \left\langle\psi(0)\middle|\hat{U}^{\dagger}(t,0)\hat{U}(t,0)\middle|\psi(0)\right\rangle\\ &= \langle\psi(0)\,|\psi(0)\rangle\end{aligned}$$

→

$$\hat{U}^{\dagger}(t,0)\hat{U}(t,0)=1$$

$$\hat{U}^{\dagger}(t,0)=U^{-1}(t,0)$$

幺正算符

将 $|\psi(t)\rangle = \hat{U}(t,0)\,|\psi(0)\rangle$ 代入到薛定谔方程中

$$i\hbar\frac{\partial}{\partial t}\left(\hat{U}(t,0)\,|\psi(0)\rangle\right) = \hat{H}\left(\hat{U}(t,0)\,|\psi(0)\rangle\right)$$

因为 $|\psi(0)\rangle$ 是任意波函数，所以有

$$\boxed{i\hbar\frac{\partial}{\partial t}\hat{U}(t,0) = \hat{H}\hat{U}(t,0)}$$

薛定谔方程

利用初始条件 $\hat{U}(0,0) = 1$ 可得

$$\hat{U}(t,0) = e^{-i\frac{\hat{H}t}{\hbar}}$$

即

$$|\psi(t)\rangle = e^{-i\frac{\hat{H}t}{\hbar}}\,|\psi(t=0)\rangle$$

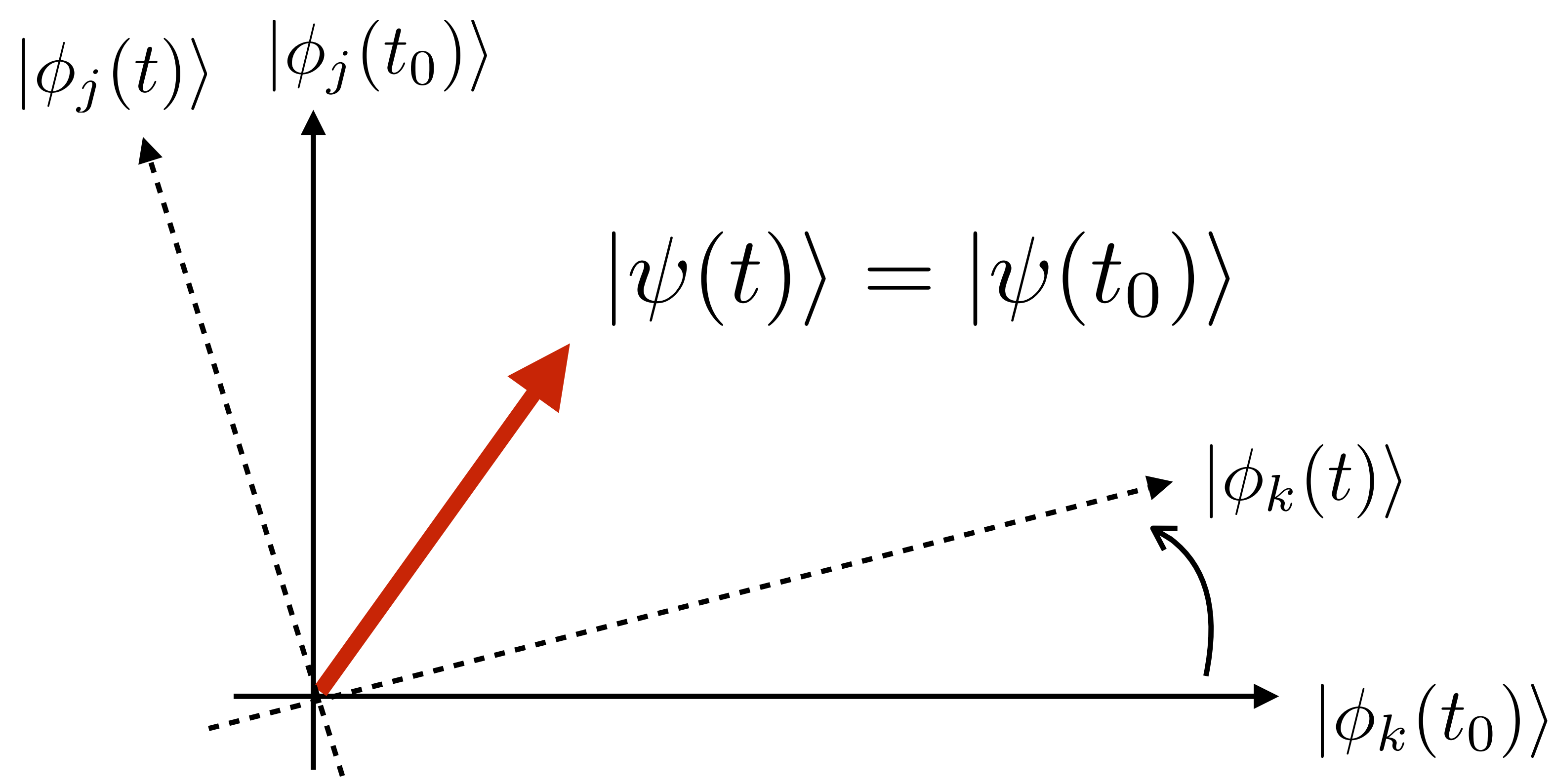
海森堡绘景

力学量平均值随时间变化

$$\begin{aligned}\langle F\rangle &= \left\langle \psi(t)\middle|\hat{F}\middle|\psi(t)\right\rangle = \left\langle \hat{U}(t,0)\psi(0)\middle|\hat{F}\middle|\hat{U}(t,0)\psi(0)\right\rangle \\ &= \left\langle \psi(0)\middle|\hat{U}^{\dagger}(t,0)\hat{F}\hat{U}(t,0)\middle|\psi(0)\right\rangle \\ &\equiv \left\langle \psi(0)\middle|\hat{F}(t)\middle|\psi(0)\right\rangle,\end{aligned}$$

$$\hat{F}(t) \equiv \hat{U}^{\dagger}(t,0)\hat{F}\hat{U}(t,0) = e^{i\frac{\hat{H}t}{\hbar}}\hat{F}e^{-i\frac{\hat{H}t}{\hbar}}$$

将力学量平均值对时间的依赖关系从波函数中提取出来，再将之置入重新定义的含时力学量算符中。



海森堡方程

$$\frac{d}{dt}\hat{F}(t) = \left(\frac{d}{dt}\hat{U}^\dagger(t,0)\right)\hat{F}\hat{U}(t,0) + \hat{U}^\dagger(t,0)\hat{F}\frac{d}{dt}\hat{U}(t,0)$$

从薛定谔方程及其共轭方程可得

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,0) = \hat{H}\hat{U}(t,0)$$

$$-i\hbar\frac{\partial}{\partial t}\hat{U}^\dagger(t,0) = \left(\hat{H}\hat{U}(t,0)\right)^\dagger = \hat{U}^\dagger(t,0)\hat{H}^\dagger = \hat{U}^\dagger\hat{H}$$

$$\begin{aligned}
\frac{d}{dt}\hat{F}(t) &= \frac{1}{-i\hbar}\left(\hat{U}^\dagger\hat{H}\right)\hat{F}\hat{U} + \hat{U}^\dagger\hat{F}\left(\frac{1}{i\hbar}\hat{H}\hat{U}\right) \\
&= \frac{1}{i\hbar}\left\{-\hat{U}^\dagger\hat{H}\hat{F}\hat{U} + \hat{U}^\dagger\hat{F}\hat{H}\hat{U}\right\} \\
&= \frac{1}{i\hbar}\left\{-\hat{U}^\dagger\hat{H}\hat{U}\hat{U}^\dagger\hat{F}\hat{U} + \hat{U}^\dagger\hat{F}\hat{U}\hat{U}^\dagger\hat{H}\hat{U}\right\} \\
&= \frac{1}{i\hbar}\left\{-\hat{H}\hat{F}(t) + \hat{F}(t)\hat{H}\right\} \\
&= \frac{1}{i\hbar}\left[\hat{F}(t),\hat{H}\right],
\end{aligned}$$

$$\hat{U}^\dagger\hat{H}\hat{U} = \hat{U}\hat{H}\hat{U}^\dagger = \hat{H}$$

$$\boxed{\frac{d}{dt}\hat{F}(t) = \frac{1}{i\hbar}\left[\hat{F}(t),\hat{H}\right]}$$

Theorem 7.2 薛定谔绘景和海森堡绘景

力学量算符

$$\hat{F}_S(t) = \hat{F}_S(0) = \hat{F}_S$$

$$\hat{F}_H(t) = e^{i\frac{\hat{H}t}{\hbar}} \hat{F}_S e^{-i\frac{\hat{H}t}{\hbar}}$$

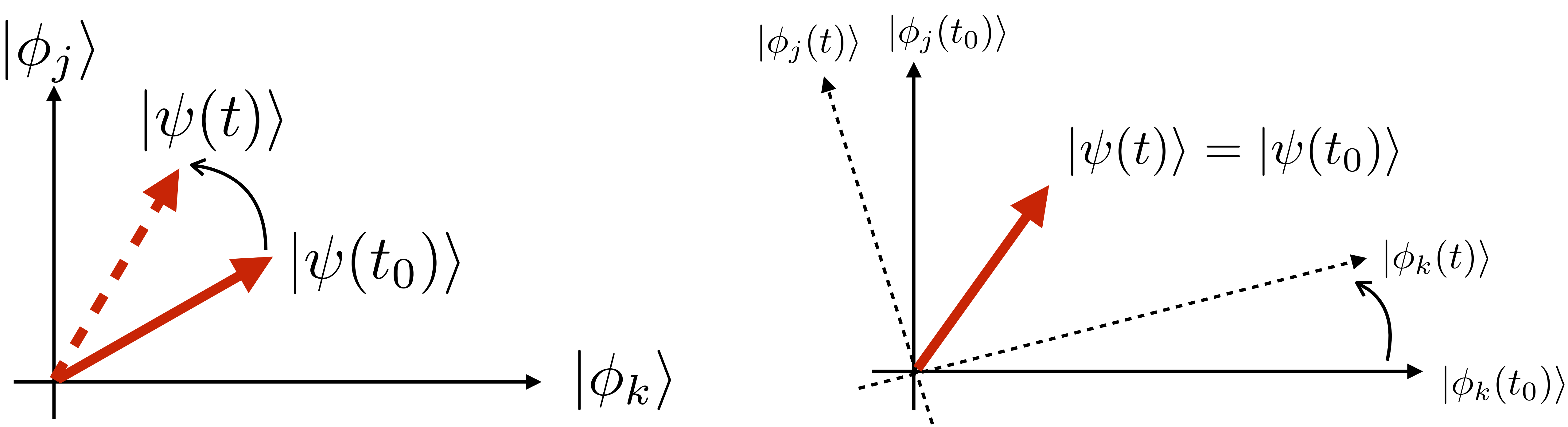
$$\frac{d}{dt}\hat{F}_H(t) = \frac{1}{i\hbar}\left[\hat{F}_H(t), \hat{H}\right]$$

态矢量

$$\psi_H(t) = \psi_H(0) = \psi_S(0) = e^{i\frac{\hat{H}t}{\hbar}} \psi_S(t)$$

$$i\hbar\frac{\partial}{\partial t}\psi_S(t) = \hat{H}\psi_S(t)$$

$$\frac{\partial}{\partial t}\psi_H(t) = 0.$$



薛定谔绘景　　海森堡绘景

狄拉克在1925

哈密顿方程 $$\frac{dx}{dt}=\frac{\partial H}{\partial p}\quad,\quad\frac{dp}{dt}=-\frac{\partial H}{\partial x}$$ $$H=\frac{p^2}{2m}+V(x)$$

设 $f(x,p,t)$ 是坐标、动量和时间的某个函数，它对时间的全导数为

$$\frac{df}{dt}=\frac{\partial f}{\partial t}+\frac{\partial f}{\partial x}\frac{\partial x}{\partial t}+\frac{\partial f}{\partial p}\frac{\partial p}{\partial t},$$

将哈密顿方程代入后得

$$\frac{df}{dt}=\frac{\partial f}{\partial t}+\{f,H\},$$

其中引入 H 和 f 的泊松括号 $\{f,H\}$:

$$\{f,H\}=\frac{\partial H}{\partial x}\frac{\partial f}{\partial p}-\frac{\partial H}{\partial p}\frac{\partial x}{\partial p}.$$

对任意的一对变量 f 和 g，泊松括号定义为

$$\{f,g\}=\frac{\partial f}{\partial x}\frac{\partial g}{\partial p}-\frac{\partial f}{\partial p}\frac{\partial g}{\partial x}$$ $$\{x,p\}=1$$

狄拉克发现：除以 $i\hbar$ 因子后的量子力学算符对易子起到和分析力学中的泊松括号类似的作用

经典	量子
$\{x, p\} = 1$	$[\hat{x}, \hat{p}] = i\hbar$
$\frac{df}{dt} = \{f, H\}$	$\frac{d\hat{f}}{dt} = \frac{1}{i\hbar}[\hat{f}, \hat{H}]$

狄拉克得到经典与量子对应原理：

将经典物理中的泊松括号替换成量子对易子并除以 $i\hbar$

1. P.A.M. Dirac, "The Fundamental Equations of Quantum Mechanics", Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 109, No. 752. (1925), pp. 642-653.