

Quantum Mechanics

量子力学

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1 形式理论

仅介绍不基于泛函分析的非严格有限维 Hilbert 空间形式理论, 默认算符的定义域为整个 Hilbert 空间.

1.1 五大公设

1.1.1 态公设

Post. 1 态矢量

- 一个量子系统的物理状态, 可由 Hilbert 空间中的一个态矢量 $|\psi\rangle \in \mathscr{H}$ 所完全描述.
- 物理状态对应的态矢量不唯一, 实际对应一个等价类 $|\psi\rangle \sim c\,|\psi\rangle$, $\forall c \in \mathbb{C}^*$.
- 通常选取归一化态矢量 $\langle\psi|\psi\rangle = 1$ 作为代表元, 而其整体相位不可观测

$$|\psi\rangle \sim \mathrm{e}^{\mathrm{i}\varphi}\,|\psi\rangle \tag{1.1}$$

1.1.2 可观测量公设

Post. 2 可观测量算符

每一个可观测量 A 均对应 Hilbert 空间上的一个自伴算符 $\hat{A} = \hat{A}^\dagger$.
从而, 记可观测量为 $\hat{A}$, 可观测量的观测值为 A.

1.1.3 测量公设

Post. 3 测量结果公设

测量可观测量 $\hat{A}$ 时, 测量结果 (measurement outcome) 一定是 $\hat{A}$ 的本征值. 有本征方程:

- 分立
  - 非简并

$$\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle \tag{1.2}$$

  - 简并

$$\hat{A}\left|a_n^{(i)}\right\rangle = a_n\left|a_n^{(i)}\right\rangle \quad (i = 1, 2, \cdots, g_n) \tag{1.3}$$

- 连续
  - 非简并

$$\hat{A}\,|a\rangle = a\,|a\rangle \tag{1.4}$$

– 简并

$$\hat{A}\,|a,r\rangle = a\,|a,r\rangle \quad (r=1,2,\cdots,g(a)) \tag{1.5}$$

其中 $|a_n\rangle$ 为属于本征值 a_n 的本征态, $|a\rangle$ 为属于本征值 a 的本征态.

Post. 4　Born 概率公设

- 若系统处于 $|\psi\rangle$ 态, 则可分别展开为

$$\begin{aligned} |\psi\rangle &\overset{\text{non-deg.}}{=\!=\!=} \sum_n c_n\,|a_n\rangle \qquad c_n = \langle a_n|\psi\rangle \\ &\overset{\text{deg.}}{=\!=\!=} \sum_{n,i} c_n^{(i)} \left|a_n^{(i)}\right\rangle \qquad c_n^{(i)} = \left\langle a_n^{(i)}\middle|\psi\right\rangle \end{aligned} \tag{1.6}$$

$$\begin{aligned} |\psi\rangle &\overset{\text{non-deg.}}{=\!=\!=} \int \mathrm{d}a\, c_a\,|a\rangle \qquad c_a = \langle a|\psi\rangle \\ &\overset{\text{deg.}}{=\!=\!=} \int \mathrm{d}a \sum_r c(a,r)\,|a,r\rangle \qquad c(a,r) = \langle a,r|\psi\rangle \end{aligned} \tag{1.7}$$

- 测得 a_n 的概率为

$$\begin{aligned} P(a_n) &\overset{\text{non-deg.}}{=\!=\!=} |c_n|^2 = |\langle a_n|\psi\rangle|^2 \\ &\overset{\text{deg.}}{=\!=\!=} \sum_{i=1}^{g_n} \left|c_n^{(i)}\right|^2 = \left|\left\langle a_n^{(i)}\middle|\psi\right\rangle\right|^2 = \langle\psi|\hat{P}_n|\psi\rangle \end{aligned} \tag{1.8}$$

其中 $\hat{P}_n = \sum_{i=1}^{g_n} \left|a_n^{(i)}\right\rangle \left\langle a_n^{(i)}\right|$ 为投影算符.

Rmk　若态矢量 $|\psi\rangle$ 未归一化, 则概率写为

$$P(a_n) = \frac{\langle\psi|\hat{P}_n|\psi\rangle}{\langle\psi|\psi\rangle} \tag{1.9}$$

- 测得 a 的概率密度为

$$\begin{aligned} \rho(a) &\overset{\text{non-deg.}}{=\!=\!=} |c(a)|^2 = |\langle a|\psi\rangle|^2 \\ &\overset{\text{deg.}}{=\!=\!=} \langle\psi|\hat{P}(a)|\psi\rangle \overset{\text{unnorm.}}{=\!=\!=} \frac{\langle\psi|\hat{P}(a)|\psi\rangle}{\langle\psi|\psi\rangle} \end{aligned} \tag{1.10}$$

其中 $\hat{P}(a) = \sum_{r=1}^{g(a)} |a,r\rangle\langle a,r|$ 为投影密度算符.

Rmk　测量值落在 a 附近 Δ 区间内的概率为

$$P(a,\Delta) = \frac{\langle\psi|\hat{P}_\Delta|\psi\rangle}{\langle\psi|\psi\rangle} \qquad \hat{P}_\Delta = \int_\Delta \mathrm{d}a\,\hat{P}(a) = \int_\Delta \mathrm{d}a \sum_{r=1}^{g(a)} |a,r\rangle\langle a,r| \tag{1.11}$$

Post. 5　坍缩公设

若测量 A 得到本征值 a_n, 则系统瞬间坍缩到对应本征态.

$$|\psi\rangle \begin{cases} \xrightarrow[\text{non-deg.}]{a_n} |a_n\rangle \\ \xrightarrow[\text{deg.}]{a_n} \dfrac{|\psi_n\rangle}{\sqrt{\langle\psi_n|\psi_n\rangle}} = \dfrac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} \end{cases} \tag{1.12}$$

$$|\psi\rangle \begin{cases} \xrightarrow[\text{non-deg.}]{a} |a\rangle \\ \xrightarrow[\text{deg.}]{a} = \dfrac{|\psi_\Delta\rangle}{\langle\psi_\Delta|\psi\Delta\rangle} = \dfrac{\hat{P}_\Delta|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_\Delta|\psi\rangle}} \end{cases} \tag{1.13}$$

1.1.4　演化公设

Post. 6　演化公设

孤立量子系统的时间演化是幺正的, 可由满足以下公理的幺正算符 $\hat{U}(t,t_0)$ 所完全描述:

1. 幺正性: $\forall t,s\in\mathbb{R}$

$$\hat{U}(t,s)\in \mathrm{U}(\mathscr{H}) = \left\{\hat{V}\in \mathrm{End}(\mathscr{H}) \mid \hat{V}^\dagger\hat{V} = \hat{V}\hat{V}^\dagger = \hat{I}\right\} \tag{1.14}$$

2. 复合性: $\forall t_2,t_1,t_0\in\mathbb{R}$,

$$\hat{U}(t_2,t_1)\hat{U}(t_1,t_0) = \hat{U}(t_2,t_0) \tag{1.15}$$

3. 连续性: $\forall|\psi\rangle\in\mathscr{H}$, $t,s,t_0,s_0\in\mathbb{R}$,

$$\lim_{\substack{t\to t_0\\ s\to s_0}} \left\|\hat{U}(t,s)|\psi\rangle - \hat{U}(t_0,s_0)|\psi\rangle\right\| = 0 \tag{1.16}$$

1.1.5　全同粒子与对称化公设

Post. 7　全同粒子

同种粒子具有不可区分性 (indistinguishability)

1.2 Hilbert 空间

1.2.1 复线性空间

Def. 1 复线性空间

设 V 为一个非空集合, 其元素称为矢量, $\mathbb{C}$ 为复数域. 若在 V 上定义加法与纯量乘法运算

$$V \times V \to V \quad (|v\rangle, |u\rangle) \mapsto |v\rangle + |u\rangle$$

$$\mathbb{C} \times V \to V \quad (c, |v\rangle) \mapsto c\,|v\rangle$$

且满足运算法则

1. 加法交换律: $\forall |v\rangle, |u\rangle \in V$,
$$|v\rangle + |u\rangle = |u\rangle + |v\rangle$$
2. 加法结合律: $\forall |v\rangle, |u\rangle, |w\rangle \in V$,
$$(|v\rangle + |u\rangle) + |w\rangle = |v\rangle + (|u\rangle + |w\rangle)$$
3. 存在零矢量: $\exists 0_V \in V$, s.t. $\forall |v\rangle \in V$,
$$|v\rangle + 0_V = 0_V + |v\rangle = |v\rangle$$
4. 加法逆元: $\forall |v\rangle \in V$, $\exists(-|v\rangle) \in V$, s.t.
$$|v\rangle + (-|v\rangle) = (-|v\rangle) + |v\rangle = 0_V$$
5. 纯量乘法的单位元: $\forall |v\rangle \in V$,
$$1_{\mathbb{C}}\,|v\rangle = |v\rangle$$
6. 纯量乘法结合律: $\forall a, b \in \mathbb{C}, |v\rangle \in V$,
$$(ab)\,|v\rangle = a(b\,|v\rangle)$$
7. 纯量加法对纯量乘法的分配律: $\forall a, b \in \mathbb{C}, |v\rangle \in V$,
$$(a+b)\,|v\rangle = a\,|v\rangle + b\,|v\rangle$$
8. 纯量乘法对矢量加法的分配律: $\forall c \in \mathbb{C}, |v\rangle, |u\rangle \in V$,
$$c(|v\rangle + |u\rangle) = c\,|v\rangle + c\,|u\rangle$$

则称 V 为复数域 $\mathbb{C}$ 上的一个线性空间, 简称复线性空间 (complex linear space).

Prop. 1　复线性空间的性质

1. V 的零元 0_V 唯一.
2. $\forall |v\rangle \in V$, $|v\rangle$ 的负元唯一.
3. $\forall |v\rangle \in V$, $0_{\mathbb{C}} |v\rangle = 0_V$.
4. $\forall c \in \mathbb{C}$, $c0_V = 0_V$.
5. $\forall c \in \mathbb{C}, |v\rangle \in V$, 若 $c |v\rangle = 0$, 则 $c = 0_{\mathbb{C}}$ 或 $|v\rangle = 0_V$.
6. $\forall |v\rangle \in V$, $(-1_{\mathbb{C}}) |v\rangle = - |v\rangle$.

1.2.2　复内积空间

Def. 2　复线性空间上的内积

设 V 为一个复线性空间. 在 V 上定义二元函数

$$\langle \ | \ \rangle : V \times V \to \mathbb{C} \quad (|v\rangle, |u\rangle) \mapsto \langle v|u\rangle$$

若 $\forall |v\rangle, |u\rangle, |w\rangle \in V$, $a, b \in \mathbb{C}$, 满足

1. 共轭对称性
$$\langle v|u\rangle = \langle u|v\rangle^*$$
2. 对第二个矢量保持线性
$$\langle v|au + bw\rangle = a \langle v|u\rangle + b \langle v|w\rangle$$
3. 正定性
$$\langle v|v\rangle \geq 0$$
且 $\langle v|v\rangle = 0$ iff $|v\rangle = 0_V$.

则称 $\langle \ | \ \rangle$ 为 V 上的一个内积 (inner product).

Prop. 2

内积对第一个矢量保持共轭线性:

$$\langle av + bu|w\rangle = a^* \langle v|w\rangle + b^* \langle u|w\rangle$$

Def. 3　复内积空间

若复线性空间 V 指定了一个内积 $\langle\,|\,\rangle$, 则称 $(V,\langle\,|\,\rangle)$ 为一个复内积空间 (complex inner product space).

Prop. 3　矢量长度

定义 $|v\rangle \in V$ 的长度为 $\||v\rangle\| = \sqrt{\langle v|v\rangle}$. $\forall c \in \mathbb{C}$, 满足

$$\|c\,|v\rangle\| = |c| \cdot \||v\rangle\|$$

Lem. 1　Cauchy-Schwarz 不等式

$\forall\, |v\rangle, |u\rangle \in V$,

$$|\langle v|u\rangle| \leq \||v\rangle\| \cdot \||u\rangle\|$$

当且仅当 $|v\rangle$ 与 $|u\rangle$ 线性相关时取等, $k \in \mathbb{C}$.

1.2.3　赋范线性空间

Def. 4　范数

设 V 为一个复线性空间. 定义正定函数

$$\|\ \| : V \to [0,\infty) \subset \mathbb{R}$$

若 $\forall\, |v\rangle, |u\rangle \in V, c \in \mathbb{C}$, 满足

1. 正定性:

$$\||v\rangle\| \geq 0$$

且 $\||v\rangle\| = 0$ iff $|v\rangle = 0_V$.

2. 绝对齐次性:

$$\|c\,|v\rangle\| = |c|\||v\rangle\|$$

3. 三角不等式:

$$\||v\rangle + |u\rangle\| \leq \||v\rangle\| + \||u\rangle\|$$

则称 $\|\ \|$ 为 V 的一个范数 (norm).

Def. 5　赋范空间

若线性空间 V 指定了一个范数 $\|\ \|$, 则称 V 为一个赋范空间 (normed space).

Prop. 4　内积诱导范数

复内积 $\langle\ |\ \rangle$ 可以诱导出范数

$$\||v\rangle\| = \sqrt{\langle v|v\rangle}$$

从而复内积空间 V 成为一个赋范空间.

1.2.4　完备性与 Hilbert 空间

Def. 6　序列收敛

设 $\{|v_n\rangle\}_{n=1}^{\infty}$ 为复内积空间 V 中的一个序列. 若存在 $|v\rangle \in V$, 使得: $\forall \epsilon > 0$, $\exists N \geq \in \mathbb{N}$, s.t. $\forall n \geq N$, $\||v_n\rangle - |v\rangle\| < \epsilon$, 则称序列 $\{|v_n\rangle\}$ 收敛 (converge) 到 $|v\rangle$, 记作 $|v_n\rangle \to |v\rangle$. 或称 $\{|v_n\rangle\}$ 有极限 $|v\rangle$, 记作

$$\lim_{n\to\infty} |v_n\rangle = |v\rangle \quad \Longleftrightarrow \quad \lim_{n\to\infty} \||v_n\rangle - |v\rangle\| = 0$$

Def. 7　Cauchy 序列

若 $\forall \epsilon > 0$, $\exists N \in \mathbb{N}$, s.t. $\forall n, m \geq N$, $\||v_n\rangle - |v_m\rangle\| < \epsilon$, 则称 $\{|v_n\rangle\}$ 为 V 中的一个 Cauchy 序列 (Cauchy sequence).

Def. 8　完备性

若 V 中每个 Cauchy 序列均有极限, 则称 V 关于其范数是完备的 (complete).

Def. 9　Hilbert 空间

若内积空间 $\mathscr{H}$ 关于其内积诱导的范数完备, 则称 $\mathscr{H}$ 为一个 Hilbert 空间 (Hilbert space).

Prop. 5

- 有限维复内积空间必定完备, 从而成为一个有限维复 Hilbert 空间.
- 无限维复内积空间不一定完备.

1.2.5　对偶空间

Def. 10　对偶矢量

设 $\mathscr{H}$ 为一个复 Hilbert 空间. 定义线性映射

$$\langle\phi| : \mathscr{H} \to \mathbb{C} \quad |\psi\rangle \mapsto \langle\phi|\psi\rangle$$

若 $\forall |\psi\rangle, |\chi\rangle \in \mathscr{H}, a, b, c \in \mathbb{C}$ 满足

1. 保持加法:
$$\langle\phi|\left(a\,|\psi\rangle+b\,|\chi\rangle\right)=a\,\langle\phi|\psi\rangle+b\,\langle\phi|\chi\rangle$$
2. 保持纯量乘法:
$$\langle\phi|\left(c\,|\psi\rangle\right)=c\,\langle\phi|\psi\rangle$$

则称 $\langle\phi|$ 为 $\mathscr{H}$ 上的一个线性泛函 (linear functional), 或称 $\langle\phi|$ 为矢量 $|\phi\rangle\in\mathscr{H}$ 的对偶矢量 (dual vector).

Rmk 也称矢量 $|\psi\rangle$ 为右矢 (ket), 对偶矢量 $\langle\psi|$ 为左矢 (bra).

Def. 11 对偶空间

$\mathscr{H}$ 中所有矢量的对偶矢量构成的集合为 $\mathbb{C}$ 上的一个复线性空间, 称为 $\mathscr{H}$ 的对偶空间 (dual space).
$$\mathscr{H}^*:=\{\langle\phi|\mid|\phi\rangle\in\mathscr{H}\}$$

1.2.6 矢量的正交与完备

Def. 12 完备正交基

- 设 $\{|u_n\rangle\}$ 为一个矢量集. 若满足
$$\langle u_n|u_m\rangle=\delta_{nm}\tag{1.17}$$
则称 $\{|u_n\rangle\}$ 为正交归一的 (orthonormal).
- 若该矢量集能张成整个 Hilbert 空间, 即该矢量集构成 $\mathscr{H}$ 的一个基, 则称 $\{|u_n\rangle\}$ 为完备的.
- 若 $\{|u_n\rangle\}$ 既是正交归一的, 又是完备的, 则称为一个完备正交基.

Prop. 6 正交归一性条件

- 分立
  - 非简并
  $$\langle a_n|a_m\rangle=\delta_{nm}\tag{1.18}$$
  - 简并
  $$\left\langle a_n^{(i)}\middle|a_m^{(j)}\right\rangle=\delta_{nm}\delta_{ij}\tag{1.19}$$
- 连续

- 非简并

$$\langle a|a'\rangle = \delta(a-a') \tag{1.20}$$

- 简并

$$\langle a,r|a',r'\rangle = \delta(a-a')\delta_{rr'} \tag{1.21}$$

Prop. 7　完备性条件

- 分立
  - 非简并

$$\sum_n |u_n\rangle\langle u_n| = \hat{I} \tag{1.22}$$

  - 简并

$$\sum_{n,i} \left|a_n^{(i)}\right\rangle \left\langle a_n^{(i)}\right| = \sum_n \hat{I}_n = \hat{I} \tag{1.23}$$

- 连续
  - 非简并

$$\int \mathrm{d}a\ |a\rangle\langle a| = \hat{I} \tag{1.24}$$

  - 简并

$$\int \mathrm{d}a \sum_{r=1}^{g(a)} |a,r\rangle\langle a,r| = \hat{I} \tag{1.25}$$

Pf　"⇒": $\forall |\psi\rangle \in \mathscr{H}$, $|\psi\rangle = \sum_n c_n |u_n\rangle$, $\langle u_m|\psi\rangle = \sum_n c_n \underbrace{\langle u_m|u_n\rangle}_{=\delta_{nm}} = c_m$,

$$\Longrightarrow |\psi\rangle = \sum_m c_m |u_m\rangle = \sum_m \langle u_m|\psi\rangle |u_m\rangle = \underbrace{\sum_m \Big(|u_m\rangle\langle u_m| \Big)}_{=\hat{I}} |\psi\rangle$$

"⇐": $|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_n |u_n\rangle\langle u_n|\right)|\psi\rangle = \sum_n \underbrace{\langle u_n|\psi\rangle}_{=c_n} |u_n\rangle$.

连续情况类似可证.

1.3 Hilbert 空间上的算符

1.3.1 线性算符

Def. 13 线性算符

若 Hilbert 空间上的一个变换 $\hat{A}:\mathscr{H}\to\mathscr{H}$ 满足

1. 保持加法: $\forall|\psi\rangle,|\phi\rangle\in\mathscr{H}$,

$$\hat{A}(|\psi\rangle+|\phi\rangle)=\hat{A}|\psi\rangle+\hat{A}|\phi\rangle$$

2. 保持纯量乘法: $\forall|\psi\rangle\in\mathscr{H},c\in\mathbb{C}$

$$\hat{A}(c|\psi\rangle)=c\hat{A}|\psi\rangle$$

则称 $\hat{A}$ 为 $\mathscr{H}$ 上的一个线性算符 (linear operator).

- 若 $\forall|\psi\rangle\in\mathscr{H}$, $\hat{A}|\psi\rangle=\hat{B}|\psi\rangle$, 则称 $\hat{A}$ 与 $\hat{B}$ 相等, 记作 $\hat{A}=\hat{B}$.
- 若 $\forall|\psi\rangle\in\mathscr{H}$, $\hat{0}|\psi\rangle=0$, 则称 $\hat{0}$ 为零算符 (zero operator).
- 若 $\forall|\psi\rangle\in\mathscr{H}$, $\hat{I}|\psi\rangle=|\psi\rangle$, 则称 $\hat{I}$ 为单位算符 (identity operator), 或恒等算符.

Thm. 1 线性算符代数

定义算符的乘法

$$(\hat{A}\hat{B})|\psi\rangle=\hat{A}\Big(\hat{B}|\psi\rangle\Big)$$

于是 $\mathscr{H}$ 上的所有算符, 对于加法、数量乘法、乘法构成一个含幺结合代数. 算符的乘法一般非交换

$$\hat{A}\hat{B}=\hat{B}\hat{A}\quad\Longleftrightarrow\quad\Big[\hat{A},\hat{B}\Big]\neq0$$

1.3.2 对易子

Def. 14 对易子

设 $\hat{A},\hat{B}$ 均为 $\mathscr{H}$ 上的线性算符, 称其对易子 (commutator) 为

$$\Big[\hat{A},\hat{B}\Big]:=\hat{A}\hat{B}-\hat{B}\hat{A}\tag{1.26}$$

若 $\Big[\hat{A},\hat{B}\Big]=0$, 则称 $\hat{A}$ 与 $\hat{B}$ 对易, 否则称其不对易.

Thm. 2　Lie 括号的公理性质

对易子 $[\ ,\ ]$ 满足 Lie 括号 (Lie bracket) 的公理化定义:

$$[\ ,\ ]:\mathrm{End}(\mathscr{H})\times\mathrm{End}(\mathscr{H})\to\mathrm{End}(\mathscr{H})$$

且 $\forall\hat{A},\hat{B},\hat{C}\in\mathrm{End}(\mathscr{H})$, $a,b\in\mathbb{C}$, 有

1. 双线性

$$\begin{aligned}\left[a\hat{A}+\hat{B},\hat{C}\right]&=a\left[\hat{A},\hat{C}\right]+b\left[\hat{B},\hat{C}\right]\\ \left[\hat{A},a\hat{B}+b\hat{C}\right]&=a\left[\hat{A},\hat{B}\right]+b\left[\hat{A},\hat{C}\right]\end{aligned}\tag{1.27}$$

2. 反对称性

$$\left[\hat{A},\hat{B}\right]=-\left[\hat{B},\hat{A}\right]\tag{1.28}$$

3. Jocobi 恒等式

$$\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0\tag{1.29}$$

从而线性算符空间 $\mathrm{End}(\mathscr{H})$ 在对易子 $[\ ,\ ]$ 下构成一个 Lie 代数 (Lie algebra).

Prop. 8　对易子的代数性质

- Leibniz 法则

$$\left[\hat{A},\hat{B}\hat{C}\right]=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right]\qquad\left[\hat{A}\hat{B},\hat{C}\right]=\hat{A}\left[\hat{B},\hat{C}\right]+\left[\hat{A},\hat{C}\right]\hat{B}\tag{1.30}$$

- 幂函数法则: 若 $\left[\hat{B},\left[\hat{A},\hat{B}\right]\right]=0$, 则

$$\left[\hat{A},\hat{B}^n\right]=n\left[\hat{A},\hat{B}\right]\hat{B}^{n-1}\tag{1.31}$$

- 函数法则: 若 $\left[\hat{B},\left[\hat{A},\hat{B}\right]\right]=0$, 则

$$\left[\hat{A},f(\hat{B})\right]=\left[\hat{A},\hat{B}\right]\frac{\partial f}{\partial\hat{B}}\tag{1.32}$$

Pf　$\left[\hat{A},\hat{B}\hat{C}\right]=\hat{A}\hat{B}\hat{C}-\hat{B}\hat{C}\hat{A}+(\hat{B}\hat{A}\hat{C}-\hat{B}\hat{A}\hat{C})=\underbrace{(\hat{A}\hat{B}-\hat{B}\hat{A})}_{=\left[\hat{A},\hat{B}\right]}\hat{C}+\hat{B}\underbrace{(\hat{A}\hat{C}-\hat{C}\hat{A})}_{=\left[\hat{A},\hat{C}\right]}$.

对幂指数 n 做数学归纳法: $n=1$, 显然成立. 设 $n=k$ 成立, 即 $\left[\hat{A},\hat{B}^n\right]=n\left[\hat{A},\hat{B}\right]\hat{B}^{n-1}$.

则对 $n=k+1$,

$$\begin{aligned}\left[\hat{A},\hat{B}^{k+1}\right]&=\hat{B}\left[\hat{A},\hat{B}^{k}\right]+\left[\hat{A},\hat{B}\right]\hat{B}^{k}=k\hat{B}\left[\hat{A},\hat{B}\right]\hat{B}^{k-1}+\left[\hat{A},\hat{B}\right]\hat{B}^{k}\\&\xlongequal{\left[\hat{B},\left[\hat{A},\hat{B}\right]\right]=0}k\left[\hat{A},\hat{B}\right]\hat{B}^{k}+\left[\hat{A},\hat{B}\right]\hat{B}^{k}=(k+1)\left[\hat{A},\hat{B}\right]\hat{B}^{k}\end{aligned}$$

命题成立, 从而对于 $n\in\mathbb{N}^*$, 幂函数法则成立.

$$\text{Let } f(\hat{B})=\sum_{n=0}^{\infty}f_n\hat{B}^n,\ \text{then } \left[\hat{A},f(\hat{B})\right]=\left[\hat{A},\sum_n f_n\hat{B}^n\right]=\sum_n f_n\hat{B}^n=\left[\hat{A},\hat{B}\right]\underbrace{\sum_n nf_n\hat{B}^{n-1}}_{=\frac{\partial f}{\partial\hat{B}}}.$$

1.3.3 指数算符与 BCH 公式

Def. 15 指数算符

算符 $\hat{A}$ 的指数算符 (exponential operator) $\mathrm{e}^{\hat{A}}$ 定义为绝对收敛的级数

$$\mathrm{e}^{\hat{A}}:=\sum_{n=0}^{\infty}\frac{\hat{A}^n}{n!}=\hat{I}+\hat{A}+\frac{\hat{A}^2}{2!}+\frac{\hat{A}^3}{3!}+\cdots \tag{1.33}$$

Prop. 9 指数算符的性质

无论算符 $\hat{A}$ 是否可逆, 均有:

- 单位算符
$$\mathrm{e}^{\hat{0}}=\hat{I} \tag{1.34}$$
- 逆算符
$$\left(\mathrm{e}^{\hat{A}}\right)^{-1}=\mathrm{e}^{-\hat{A}} \tag{1.35}$$
- 对参数的导数
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{t\hat{A}}=\hat{A}\mathrm{e}^{t\hat{A}}=\mathrm{e}^{t\hat{A}}\hat{A} \tag{1.36}$$
- 迹
$$\det\left(\mathrm{e}^{\hat{A}}\right)=\mathrm{e}^{\operatorname{tr}\hat{A}} \tag{1.37}$$

Pf $\mathrm{e}^{0\hat{0}}=\hat{I}+\hat{0}+\cdots=\hat{I}$.

Prop. 10

若 $\left[\hat{A},\hat{B}\right]=0$, 则

$$\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}=\mathrm{e}^{\hat{A}+\hat{B}} \tag{1.38}$$

Lem. 2　Baker-Hausdorff 引理

共轭变换 $\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}}$ 可展开为级数

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right] + \frac{1}{2!}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \cdots + \left[\hat{A},\left[\hat{A},\cdots\left[\hat{A},\hat{B}\right]\cdots\right]\right]^{(n)} + \cdots \tag{1.39}$$

若定义对易子映射

$$\mathrm{ad}_{\hat{A}} : \hat{B} \mapsto \left[\hat{A},\cdot\right](\hat{B}) = \left[\hat{A},\hat{B}\right] \tag{1.40}$$

则可将 BH 引理写为

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}} = \sum_{n=0}^{\infty}\frac{\mathrm{ad}_{\hat{A}}(\hat{B})}{n!} \tag{1.41}$$

Thm. 3　Baker-Compbell-Hausdorff 公式

$$\ln\left(\mathrm{e}^{\hat{A}}\hat{B}\right) = \hat{A} + \hat{B} + \frac{1}{2}\left[\hat{A},\hat{B}\right] + \frac{1}{12}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] - \frac{1}{12}\left[\hat{B},\left[\hat{A},\hat{B}\right]\right] + \cdots \tag{1.42}$$

Cor. 1　2 阶截断的 BCH 公式

$$\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} = \mathrm{e}^{\hat{A}+\hat{B}}\mathrm{e}^{\frac{1}{2}\left[\hat{A},\hat{B}\right]} \qquad \mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{-\frac{1}{2}\left[\hat{A},\hat{B}\right]} \tag{1.43}$$

Cor. 2　对易情形

若 $\hat{A}$ 与 $\hat{B}$ 对易, 即 $\left[\hat{A},\hat{B}\right] = 0$, 则有

$$\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} = \mathrm{e}^{\hat{A}+\hat{B}} \tag{1.44}$$

1.3.4　本征值与本征矢

Def. 16　本征值, 本征矢, 本征态, 本征空间, 简并度

- 对于 $a \in \mathbb{C}$, 若存在 $|a\rangle \in \mathscr{H} \setminus \{0\}$ 使得 $\hat{A}|a\rangle = a|a\rangle$, 则称 a 为 $\hat{A}$ 的本征值 (eigenvalue), 称 $|a\rangle$ 为 $\hat{A}$ 的属于本征值 a 的本征矢 (eigenvector).
- 与本征矢对应的量子态, 称为本征态 (eigenstate).
- 称由 a 的所有本征矢张成的空间

  $$\mathscr{E}_a := \{|a\rangle \in \mathscr{H} \mid \hat{A}|a\rangle = a|a\rangle\} \cup \{0\}$$

  为 a 的本征子空间 (eigensubspace).

- 本征空间的维数, 称为本征值 a 的简并度 (degeneracy).

$$g_a := \dim \mathscr{E}_a$$

  - 若 $g = 1$, 则称 a 非简并 (non-degenerate).
  - 若 $g > 1$, 则称 a 简并 (degenerate).

Thm. 4　谱分解

$$\mathscr{H} = \bigoplus_a \mathscr{E}_a \tag{1.45}$$

Def. 17　谱

- 设 $\hat{A}$ 为量子系统的一个可观测量. $\hat{A}$ 的所有本征值构成的集合, 称为 $\hat{A}$ 的本征谱 (eigenspectrum), 记作 $\mathrm{Spec}(\hat{A})$,
- 若可观测量的谱值可以由离散指标记为 $\{a_1, a_2, \cdots, a_n, \cdots\}$

Def. 18　离散谱与连续谱

1.3.5　外积与投影算符

Def. 19　外积算符

$\forall |\psi\rangle, |\phi\rangle \in \mathscr{H}$, 其外积 $|\psi\rangle\langle\phi|$ 可定义一个线性算符: $\forall |\chi\rangle \in \mathscr{H}$,

$$\big(|\phi\rangle\langle\phi|\big)|\chi\rangle = \big(\langle\phi|\chi\rangle\big)|\psi\rangle \tag{1.46}$$

Def. 20　投影算符

若线性算符 $\hat{P}$ 满足

1. 幂等性 (idempotency)

$$\hat{P}^2 = \hat{P} \tag{1.47}$$

2. 自伴性

$$\hat{P}^\dagger = \hat{P} \tag{1.48}$$

则称 $\hat{P}$ 为一个正交投影算符 (orthogonal projection operator).
若 $|\psi\rangle \in \mathscr{H}$ 归一, 则可定义向 $|\psi\rangle$ 方向的投影算符

$$\hat{P}_\psi = |\psi\rangle\langle\psi| \tag{1.49}$$

易证 $\hat{P}_\psi$ 为一个正交投影算符.

Rmk 只满足幂等性, 而不要求自伴性的算符, 称为投影算符.

Prop. 11 投影算符的本征值问题

投影算符 $\hat{P}_\psi$ 的本征值只有 $0,1$ 两个取值, 分别对应两个本征矢 $|0\rangle, |1\rangle$. 分别称其为正交态 (orthogonal state) $|\psi_\perp\rangle = |0\rangle$ 与平行态 (parallel state) $\left|\psi_\parallel\right\rangle = |1\rangle$.

Prop. 12 任意态矢量的正交投影分解

$\forall |\phi\rangle \in \mathscr{H}$, $|\phi\rangle = |\phi_\perp\rangle + \left|\phi_\parallel\right\rangle$.

$$\begin{cases} |\phi_\perp\rangle = (\hat{I} - \hat{P}_\psi)|\phi\rangle \\ \left|\phi_\parallel\right\rangle = \hat{P}_\psi |\phi\rangle \end{cases} \tag{1.50}$$

其中 $|\phi_\perp\rangle, \left|\phi_\parallel\right\rangle$ 分别为 $\hat{P}_\psi$ 的属于本征值 $0,1$ 的本征矢, 即

$$\hat{P}_\psi |\phi_\perp\rangle = 0 \qquad \hat{P}_\psi \left|\phi_\parallel\right\rangle = \left|\phi_\parallel\right\rangle \tag{1.51}$$

Pf $\left\langle\phi_\perp\middle|\phi_\parallel\right\rangle = \langle\phi|(\hat{I} - \hat{P}_\psi)^\dagger \hat{P}_\psi |\phi\rangle = \langle\phi| \underbrace{(\hat{P}_\psi - \hat{P}_\psi^2)}_{=0} |\phi\rangle = 0$

Def. 21 本征子空间的投影算符

设 $\hat{A}$ 有简并的本征值 a, 即 $\hat{A}\left|a^{(i)}\right\rangle = a\left|a^{(i)}\right\rangle$, $i = 1, \cdots, g_a$. 则定义 a 的本征子空间的投影算符为

$$\hat{P}_a = \sum_{i=1}^{g_a} \left|a^{(i)}\right\rangle \left\langle a^{(i)}\right| \tag{1.52}$$

1.3.6 自伴算符与反自伴算符

Def. 22 伴随算符

$\forall |\psi\rangle, |\phi\rangle \in \mathscr{H}$, 有内积关系

$$\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\phi\rangle^* \tag{1.53}$$

称 $\hat{A}^\dagger$ 为线性算符 $\hat{A}$ 的伴随 (adjoint).

Def. 23 自伴算符

若线性算符 $\hat{A}$ 的伴随算符等于其自身, 即

$$\hat{A}^\dagger = \hat{A} \tag{1.54}$$

则称 $\hat{A}$ 为一个自伴算符 (self-adjoint operator).

Rmk 无限维 Hilbert 空间中, 自伴算符还要求定义域

$$D(\hat{A}) = D(\hat{A}^\dagger) \tag{1.55}$$

因此有限维 Hilbert 空间中, 对称算符 $\langle\phi|\,\hat{A}\,|\psi\rangle = \langle\psi|\,\hat{A}\,|\phi\rangle^*$ 与自伴算符没有分别, 而在无限维 Hilbert 空间中, 可观测量对应的只能是自伴算符.

Thm. 5 自伴算符的本征值

自伴算符 $\hat{A}$ 的本征值必为实值, 即

$$\hat{A}\,|a\rangle = a\,|a\rangle \quad \Longrightarrow \quad a \in \mathbb{R} \tag{1.56}$$

Pf $\langle a|\hat{A}|a\rangle = a\,\langle a|a\rangle = \langle a|\hat{A}^\dagger|a\rangle = (a\,|a\rangle)^\dagger\,|a\rangle = a^*\,\langle a|a\rangle, \implies a = a^*.$

Thm. 6 自伴算符的谱定理

自伴算符的所有本征子空间的直和, 即为 Hilbert 空间. 从而自伴算符的本征矢, 可以构成一个完备正交基.

Def. 24 反自伴算符

若线性算符 $\hat{A}$ 满足

$$\hat{A}^\dagger = -\hat{A} \tag{1.57}$$

则称为一个反自伴算符 (anti-self-adjoint operator).

Prop. 13 反自伴算符的本征值

反自伴算符 $\hat{A}$ 的本征值必为纯虚值, 即

$$\hat{A}\,|a\rangle = \mathrm{i}a\,|a\rangle \quad (a \in \mathbb{R}) \tag{1.58}$$

Pf $\langle a|\hat{A}|a\rangle = \mathrm{i}a\,\langle a|a\rangle = -\,\langle a|\hat{A}^\dagger|a\rangle = -(\mathrm{i}a\,|a\rangle)^\dagger\,|a\rangle = \mathrm{i}a^*\,\langle a|a\rangle, \implies a = a^*.$

Prop. 14 对易子的反自伴性

若 $\hat{A}$ 与 $\hat{B}$ 均为自伴算符, 则 $\left[\hat{A}, \hat{B}\right]$ 为一个反自伴算符. 可写为

$$\left[\hat{A}, \hat{B}\right] = \mathrm{i}\hat{C} \tag{1.59}$$

其中 $\hat{C}$ 为一个自伴算符.

Prop. 15　算符的自伴-反自伴分解

任意一个算符 $\hat{O}$, 均可以分解为自伴算符与斜自伴算符之和.

$$\hat{O} = \frac{1}{2}\left(\hat{O} + \hat{O}^\dagger\right) + \frac{1}{2}\left(\hat{O} - \hat{O}^\dagger\right) \tag{1.60}$$

其中 $\frac{1}{2}\left(\hat{O} + \hat{O}^\dagger\right)$ 为自伴算符, $\frac{1}{2}\left(\hat{O} - \hat{O}^\dagger\right)$ 为斜自伴算符.

1.4　幺正变换

1.4.1　幺正算符的代数性质

Def. 25　幺正算符

若 $\hat{U}$ 为可逆线性算符, 且满足

$$\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{I} \quad \Longleftrightarrow \quad \hat{U}^\dagger = \hat{U}^{-1} \tag{1.61}$$

则称 $\hat{U}$ 为幺正算符.

Thm. 7　保内积性质

幺正算符不改变态矢量之间的内积. 设 $|\psi\rangle \to |\psi'\rangle = \hat{U}|\psi\rangle$, $|\phi\rangle \to |\phi'\rangle = \hat{U}|\phi\rangle$. 则

$$\langle\phi'|\psi'\rangle = \langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle \tag{1.62}$$

Prop. 16　等效算符变换

若态矢量进行主动变换 $|\psi'\rangle = \hat{U}|\psi\rangle$, 可观测量不变, 则可将态矢量上的变换转移到算符上:

$$\hat{A}_{\text{eff}} = \hat{U}^\dagger\hat{A}\hat{U} \tag{1.63}$$

在等效下, 可观测量 $\hat{A}$ 的测量期望值不变.

$$\langle\psi'|\hat{A}|\psi'\rangle = \langle\psi|\underbrace{\hat{U}^\dagger\hat{A}\hat{U}}_{=A_{\text{eff}}}|\psi\rangle \tag{1.64}$$

Rmk

Prop. 17　算符的主动变换

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger \tag{1.65}$$

Prop. 18　幺正算符的本征值

对于 $\hat{U}\left|u\right\rangle = u\left|u\right\rangle$, $\left|u\right\rangle \neq 0$, 有

$$|u| = 1 \qquad u = \mathrm{e}^{\mathrm{i}\theta} \quad (\theta \in \mathbb{R}) \tag{1.66}$$

即, 幺正算符的本征值位于复平面的单位圆上.

Thm. 8　幺正群

Hilbert 空间 $\mathscr{H}$ 上所有幺正算符对于映射的复合构成一个群, 称为幺正群 (unitary group).

$$\mathrm{U}(\mathscr{H}) := \left\{\hat{U} \in \mathrm{GL}(\mathscr{H}) \mid \hat{U}^\dagger = \hat{U}^{-1}\right\} \tag{1.67}$$

$\mathrm{U}(\mathscr{H})$ 中所有行列式为 1 的算符也构成一个群, 称为特殊幺正群 (special unitary group).

$$\mathrm{SU}(\mathscr{H}) := \left\{\hat{U} \in \mathrm{U}(\mathscr{H}) \mid \det \hat{U} = 1\right\} \tag{1.68}$$

Thm. 9　三性合一

以下算符的三种性质中, 任意两个成立时, 第三个必成立:

1. 自伴性: $\hat{A}^\dagger = \hat{A}$;
2. 幺正性: $\hat{A}^\dagger = \hat{A}^{-1}$;
3. 对合性: $\hat{A}^2 = \hat{I}$.

此时算符的本征值必为 1 或 -1.

Pf　$\hat{A}^2\left|a\right\rangle = a\hat{A}\left|a\right\rangle = a^2\left|a\right\rangle = \left|a\right\rangle$, $\Longrightarrow$ $a \in \{\pm 1\}$.

1.4.2　指数形式与 Lie 群

1.4.3　无穷小变换与 Lie 代数

1.5　表象

Def. 26　表象

在 Hilbert 空间中选定一个完备正交基, 称由此基建立的一个坐标系, 为一个表象 (representation). 可观测量 $\hat{A}$ 的本征矢 $\{\left|a\right\rangle\}$ 构成一个完备正交基, 从而建立 $\hat{A}$-表象, 称为 $\hat{A}$ 的本征表象 (eigenrepresentation), 或称 $\{\left|a\right\rangle\}$-表象.

1.5.1 波函数

Def. 27 波函数

态矢量在一个表象下的展开系数, 称为波函数 (wavefunction).

Prop. 19 分立表象下的波函数

在 $\{|a_n\rangle\}$-表象下, 态矢量 $|\psi\rangle$ 展开为

$$|\psi\rangle = \sum_n \underbrace{\langle a_n|\psi\rangle}_{=c_n} |a_n\rangle \tag{1.69}$$

其中 $c_n = \langle a_n|\psi\rangle$ 称为 $|\psi\rangle$ 在 $\{|a_n\rangle\}$-表象下的波函数的第 n 个分量.

Prop. 20 连续表象下的波函数

在 $\{|a\rangle\}$-表象下, 态矢量 $|\psi\rangle$ 展开为

$$|\psi\rangle = \int \mathrm{d}a \underbrace{\langle a|\psi\rangle}_{=c(a)} |a\rangle \tag{1.70}$$

其中 $c(a) = \langle a|\psi\rangle$ 称为 $|\psi\rangle$ 在 $\{|a\rangle\}$-表象下的波函数.

1.5.2 算符在表象下的矩阵表示

Thm. 10 算符的矩阵表示

选定表象 $\{|u_n\rangle\}$, 算符 $\hat{A}$ 在该表象下的矩阵表示为

$$\hat{A}(|u_1\rangle, |u_2\rangle, \cdots, |u_n\rangle, \cdots) = (|u_1\rangle, |u_2\rangle, \cdots, |u_n\rangle, \cdots)\boldsymbol{A} \tag{1.71}$$

$\boldsymbol{A}$ 的矩阵元为

$$A_{nm} = \langle u_n|\hat{A}|u_m\rangle \tag{1.72}$$

Pf 将算符写为外积展开的形式

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left(\sum_n |u_n\rangle\langle u_n|\right)\hat{A}\left(\sum_m |u_m\rangle\langle u_m|\right) = \sum_{nm} \underbrace{\langle u_n|\hat{A}|u_m\rangle}_{=A_{nm}} |u_n\rangle\langle u_m|$$

Thm. 11 *

非简并算符 $\hat{A}$ 在自身表象下的矩阵为对角矩阵

$$\hat{A} = \mathrm{diag}(a_1, \cdots, a_n) \tag{1.73}$$

Def. 28　算符的迹

算符在一个表象下的矩阵的迹, 称为算符的迹 (trace).

Pf　$\operatorname{tr}\hat{A} = \sum_{n,m} A_{nm} \underbrace{\operatorname{tr}(|u_n\rangle\langle u_m|)}_{=\delta_{nm}} = \sum_n A_{nn}.$

Prop. 21　迹的性质

$$\operatorname{tr}(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle \tag{1.74}$$

$$\operatorname{tr}\left(\hat{A}\hat{B}\right) = \operatorname{tr}\left(\hat{B}\hat{A}\right) \tag{1.75}$$

$$\operatorname{tr}\left(\hat{A}_1\hat{A}_2\cdots\hat{A}_n\right) = \operatorname{tr}\left(\hat{A}_2\cdots\hat{A}_n\hat{A}_1\right) = \operatorname{tr}\left(\cdots\hat{A}_n\hat{A}_1\hat{A}_2\right) \tag{1.76}$$

Prop. 22　伴随的矩阵表示

在一个表象下, $\boldsymbol{A}^\dagger$ 为 $\boldsymbol{A}$ 的复共轭转置矩阵 (complex conjugate transpose)

$$(\boldsymbol{A}^\dagger)_{ij} = A^*_{ji} \tag{1.77}$$

1.5.3　表象变换

Thm. 12　基矢变换

基 $\{u_n\}$ 到 $\{v_n\}$ 的变换为

$$|v_n\rangle = \hat{S}\,|u_n\rangle \tag{1.78}$$

其中 $\hat{S}$ 称为表象变换算符 (representation transformation operator).

$$\hat{S} = \sum_m |v_m\rangle\langle u_m| \tag{1.79}$$

$\hat{S}$ 与 $\hat{S}^\dagger$ 的矩阵元分别为

$$\langle u_k|\hat{S}|u_l\rangle = \langle v_k|\hat{S}|v_l\rangle = \langle u_k|v_l\rangle \tag{1.80}$$

$$\langle u_k|\hat{S}^\dagger|u_l\rangle = \langle v_k|\hat{S}^\dagger|v_l\rangle = \langle v_k|u_l\rangle \tag{1.81}$$

Pf　$|v_n\rangle = \sum_m |u_m\rangle \underbrace{\langle u_m|v_n\rangle}_{:=S_{mn}} = \sum_m u_m\langle u_m|\hat{S}|u_n\rangle = \underbrace{\left(\sum_m |u_m\rangle\langle u_m|\right)}_{=\hat{I}}\hat{S}\,|u_n\rangle.$

Thm. 13　表象变换算符

表象变换算符 $\hat{S}$ 是个幺正算符

$$\hat{S}^\dagger = \hat{S}^{-1} \quad\Longleftrightarrow\quad \hat{S}^\dagger\hat{S} = \hat{S}\hat{S}^\dagger = \hat{I} \tag{1.82}$$

Rmk 表象变换不改变 Hilbert 空间的度量性质, 从而不改变量子系统的物理内容, 只改变数学描述的方式.

Cor. 3 逆变换

$$|u_n\rangle = \hat{S}^\dagger |v_n\rangle \tag{1.83}$$

Prop. 23 分量变换

设 $|\psi\rangle = \sum_n c_n |u_n\rangle = \sum_m d_m |v_m\rangle$, $c_n = \langle u_n|\psi\rangle$, $d_m = \langle v_m|\psi\rangle$. 态矢量的分量变换为

$$d_m = \sum_n S^*_{nm} c_n = \sum_n (\boldsymbol{S}^\dagger)_{mn} c_n \quad \Longleftrightarrow \quad \boldsymbol{d} = \boldsymbol{S}^\dagger \boldsymbol{c} \tag{1.84}$$

Prop. 24 算符变换

$$\hat{A}_v = \hat{S}^\dagger \hat{A}_u \hat{S} \tag{1.85}$$

Pf $(\hat{A}_v)_{kl} = \langle v_k|\hat{A}|v_l\rangle$, $(\hat{A}_u)_{kl} = \langle u_n|\hat{A}|u_m\rangle$.

$$\begin{aligned}\langle v_k|\hat{A}|v_l\rangle &= \sum_{n,m} \langle v_k|u_n\rangle \langle u_n|\hat{A}|u_m\rangle \langle u_m|v_l\rangle = \sum_{n,m} \langle u_k|\hat{S}^\dagger|u_n\rangle \langle u_n|\hat{A}|u_m\rangle \langle u_m|\hat{S}|u_l\rangle \\ &= \langle u_k| \hat{S}^\dagger \left(\sum_n |u_n\rangle \langle u_n|\right) \hat{A} \left(\sum_m |u_m\rangle \langle u_m|\right) \hat{S} |u_l\rangle = \langle u_k|\hat{S}^\dagger \hat{A} \hat{S}|u_l\rangle\end{aligned}$$

1.5.4 位置表象与动量表象

Thm. 14 $\hat{x}$ 与 $\hat{p}$ 在 $\hat{x}$-表象下的表示

$$\hat{\boldsymbol{x}} = \boldsymbol{x} \qquad \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla \tag{1.86}$$

$$\hat{x}_i = x_i \qquad \hat{p}_i = -\mathrm{i}\hbar \frac{\partial}{\partial x_i} \tag{1.87}$$

Prop. 25 位置表象的本征方程与完备正交性条件

$$\hat{\boldsymbol{x}} |\boldsymbol{x}\rangle = \boldsymbol{x} |\boldsymbol{x}\rangle \tag{1.88}$$

$$\langle \boldsymbol{x}|\boldsymbol{x}'\rangle = \delta(\boldsymbol{x} - \boldsymbol{x}') \tag{1.89}$$

$$\int \mathrm{d}^3 x \ |\boldsymbol{x}\rangle \langle \boldsymbol{x}| = \hat{I} \tag{1.90}$$

Prop. 26　动量表象的完备正交性条件

$$\hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\,|\boldsymbol{p}\rangle \tag{1.91}$$

$$\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}') \tag{1.92}$$

$$\int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\,\langle \boldsymbol{p}| = \hat{I} \tag{1.93}$$

Thm. 15　位置表象与动量表象下的波函数

$$\psi(\boldsymbol{x}) = \langle \boldsymbol{x}|\psi\rangle \tag{1.94}$$

$$\tilde{\psi}(\boldsymbol{p}) = \langle \boldsymbol{p}|\psi\rangle \tag{1.95}$$

Thm. 16　表象变换

1.6　可观测量算符

1.6.1　$\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}, \hat{\boldsymbol{L}}$ 间的对易关系

Post. 8　基本对易关系

将经典力学基本 Poisson 括号 $[x_i, x_j]_{\mathrm{PB}} = [p_i, p_j]_{\mathrm{PB}} = 0$, $[x_i, p_j]_{\mathrm{PB}} = \delta_{ij}$ 经正则量子化替换

$$[A, B]_{\mathrm{PB}} \longleftrightarrow \frac{1}{\mathrm{i}\hbar}\big[\hat{A}, \hat{B}\big] \tag{1.96}$$

可得量子力学的基本对易关系 (fundamental commutation relations)

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \tag{1.97}$$

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}\hat{I} \tag{1.98}$$

Def. 29　轨道角动量的算符表示

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}} \quad \Longleftrightarrow \quad \hat{L}_i = \varepsilon_{ijk}\hat{x}_j\hat{p}_k \tag{1.99}$$

Prop. 27　轨道角动量相关的对易关系

$$\big[\hat{L}_i, \hat{x}_j\big] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{x}_k \tag{1.100}$$

$$\big[\hat{L}_i, \hat{p}_j\big] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{p}_k \tag{1.101}$$

$$\big[\hat{L}_i, \hat{L}_j\big] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k \quad \Longleftrightarrow \quad \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = \mathrm{i}\hbar\hat{\boldsymbol{L}} \tag{1.102}$$

$$\left[\hat{\boldsymbol{L}}^2, \hat{L}_i\right] = 0 \tag{1.103}$$

1.6.2 相容可观测量与量子数

Def. 30 相容可观测量

若可观测量 $\hat{A}, \hat{B}$ 对应的算符对易, 即

$$\left[\hat{A}, \hat{B}\right] = 0 \tag{1.104}$$

则称 A 与 B 为相容可观测量 (compatible observable).

Cor. 4

若 $\hat{A}$ 与 $\hat{B}$ 相容, 则 $\hat{A}$ 与 $f(\hat{B})$ 也相容.

Pf 由对易子的函数法则可得.

Thm. 17 相容可观测量定理

可观测量 $\hat{A}$ 与 $\hat{B}$ 相容 $\Longleftrightarrow$ $\hat{A}$ 与 $\hat{B}$ 有共同本征态集合 (set of common eigenstates), 且其构成一个正交完备基, 称为共同本征表象 (simultaneous eigenrepresentation). $\hat{A}$ 与 $\hat{B}$ 在共同本征表象下可同时对角化, 亦即可同时有确定值.

$$\hat{A}\left|a,b\right\rangle = a\left|a,b\right\rangle \qquad \hat{B}\left|a,b\right\rangle = b\left|a,b\right\rangle \tag{1.105}$$

Pf "$\Leftarrow$": 若存在共同本征表象 $\{|a,b\rangle\}$, $\hat{A}$ 与 $\hat{B}$ 可同时对角化, $\Longrightarrow$ $\left[\hat{A}, \hat{B}\right] = 0$.
"$\Rightarrow$": 以分立情况为例, 设 $\hat{A}\left|a_n^{(i)}\right\rangle = a_n\left|a_n^{(i)}\right\rangle$, $i = 1, 2, \cdots, g_n$. 则

$$\begin{cases} \left\langle a_n^{(i)}\middle|\hat{A}\hat{B}\middle|a_m^{(j)}\right\rangle = a_n\left\langle a_n^{(i)}\middle|\hat{B}\middle|a_m^{(j)}\right\rangle \\ \left\langle a_n^{(i)}\middle|\hat{B}\hat{A}\middle|a_m^{(j)}\right\rangle = a_m\left\langle a_n^{(i)}\middle|\hat{B}\middle|a_m^{(j)}\right\rangle \end{cases} \xrightarrow{a_n \neq a_m} \left\langle a_n^{(i)}\middle|\hat{B}\middle|a_m^{(j)}\right\rangle = 0$$

从而 $\hat{B}$ 为块对角

Def. 31 相容可观测量完备集

(complete set of compatible observables)

Def. 32 量子数

1.6.3 期望值与方差

Def. 33 期望值

可观测量 $\hat{A}$ 的期望值 (expectation value) 为

$$\left\langle \hat{A} \right\rangle \overset{\text{norm.}}{=\!=} \langle\psi|\hat{A}|\psi\rangle \overset{\text{unnorm.}}{=\!=} \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{1.106}$$

Rmk $\left\langle \hat{A} \right\rangle$ 由 $|\psi\rangle$ 决定, 反映了系统的量子态.

Pf $\left\langle \hat{A} \right\rangle = \sum_n P(a_n)a_n = \sum_n \langle\psi|a_n\rangle \langle a_n|\psi\rangle a_n = \langle\psi| \left(\sum_n |a_n\rangle \langle a_n| \hat{A} \right) |\psi\rangle = \langle\psi|\hat{A}|\psi\rangle.$

Prop. 28 自伴算符与反自伴算符的期望值

自伴算符的期望值为实值, 反自伴算符的期望值为纯虚值.

Def. 34 均方差

定义可观测量 $\hat{A}$ 的偏差算符 (deviation operator) 为

$$\Delta\hat{A} = \hat{A} - \left\langle \hat{A} \right\rangle \hat{I} \tag{1.107}$$

则均方差 (variance) 为

$$(\Delta A)^2 := \left\langle \left(\Delta\hat{A}\right)^2 \right\rangle = \left\langle \left(\hat{A} - \left\langle \hat{A} \right\rangle \hat{I}\right)^2 \right\rangle = \left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2 \tag{1.108}$$

标准差 (stand deviation) 或称均方根 (root mean square, rms) 为

$$\Delta A = \sqrt{(\Delta A)^2} = \sqrt{\left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2} \tag{1.109}$$

Rmk 均方差更细致地反映了系统的量子态.

Prop. 29 偏差算符的性质

- 自伴性

$$\Delta\hat{A}^\dagger = \Delta\hat{A} \qquad \Longrightarrow \Delta\hat{A}^2 = \left(\Delta\hat{A}\right)^\dagger \Delta\hat{A} \tag{1.110}$$

- 对易子

$$\left[\Delta\hat{A}, \Delta\hat{B}\right] = \left[\hat{A}, \hat{B}\right] \tag{1.111}$$

- 与标准差的关系

$$\Delta A^2 = \left\langle \Delta\hat{A}^2 \right\rangle \tag{1.112}$$

1.6.4 不确定性关系

Thm. 18 Robertson 不确定性关系

$$\Delta A\Delta B \geq \frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right| \tag{1.113}$$

Pf $\left\langle\Delta\hat{A}^2\right\rangle = \langle\psi|\Delta\hat{A}^\dagger\Delta\hat{A}|\psi\rangle =: \langle\psi_A|\psi_A\rangle$, 同理 $\left\langle\Delta\hat{B}^2\right\rangle = \langle\psi_B|\psi_B\rangle$. 由 Cauchy-Schwarz 不等式可得

$$\begin{aligned}\Delta A^2\Delta B^2 &= \left\langle\Delta\hat{A}^2\right\rangle\left\langle\Delta\hat{B}^2\right\rangle = \langle\psi_A|\psi_A\rangle\langle\psi_B|\psi_B\rangle \geq |\langle\psi_A|\psi_B\rangle|^2 = \left|\langle\psi|\Delta\hat{A}^\dagger\Delta\hat{B}|\psi\rangle\right|^2\\ &= \left|\langle\psi|\Delta\hat{A}\Delta\hat{B}|\psi\rangle\right|^2 = \left|\left\langle\Delta\hat{A}\Delta\hat{B}\right\rangle\right|^2 = \left|\left\langle\frac{1}{2}\left[\Delta\hat{A},\Delta\hat{B}\right]+\frac{1}{2}\left\{\Delta\hat{A},\Delta\hat{B}\right\}\right\rangle\right|^2\\ &= \frac{1}{4}\left|\left\langle\left[\Delta\hat{A},\Delta\hat{B}\right]\right\rangle\right|^2+\frac{1}{4}\left|\left\langle\left\{\Delta\hat{A},\Delta\hat{B}\right\}\right\rangle\right|^2 \geq \frac{1}{4}\left|\left\langle\left[\Delta\hat{A},\Delta\hat{B}\right]\right\rangle\right|^2 = \frac{1}{4}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|^2\end{aligned}$$

Thm. 19 Schrödinger-Robertson 不确定性关系

$$\Delta A\Delta B \geq \frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right| + \frac{1}{2}\left\langle\left\{\Delta\hat{A},\Delta\hat{B}\right\}\right\rangle \tag{1.114}$$

Cor. 5 Heisenberg 不确定性关系

$$\Delta x\Delta p \geq \frac{\hbar}{2} \tag{1.115}$$

Pf 在 Robertson 不确定性关系中, 取 $\hat{A}=\hat{x}$, $\hat{B}=\hat{p}$, $\left[\hat{A},\hat{B}\right]=[\hat{x},\hat{p}]=\mathrm{i}\hbar$, 由此可得.

1.6.5 密度算符

若由于缺乏系统的信息, 导致无法确定其状态, 而该种不确定性并非由量子力学的内禀不确定性导致, 从而可用系综描述这种经典统计力学的不确定性.

Def. 35 密度算符

若系统处在 $|\psi_i\rangle$ 态的经典概率为 p_i, 则可定义密度算符 (density operator)

$$\hat{\rho} = \sum_i p_i\,|\psi_i\rangle\langle\psi_i| \tag{1.116}$$

若系统处在 $|\psi(\lambda)\rangle$ 态的经典概率密度为 $f(\lambda)$, 则密度算符为

$$\hat{\rho} = \int \mathrm{d}\lambda\, f(\lambda)\,|\psi(\lambda)\rangle\langle\psi(\lambda)| \tag{1.117}$$

Thm. 20　密度算符形式的期望值公式

$$\left\langle \hat{A} \right\rangle_{\rho} = \mathrm{tr}\left(\hat{\rho}\hat{A}\right) \tag{1.118}$$

Pf　Discrete: $\mathrm{tr}\left(\hat{\rho}\hat{A}\right) = \mathrm{tr}\left(\sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| \hat{A}\right) = \sum_i p_i \,\mathrm{tr}\left(\left\langle\psi_i\right|\hat{A}\left|\psi_i\right\rangle\right) = \sum_i p_i \left\langle\psi_i\right|\hat{A}\left|\psi_i\right\rangle$

Prop. 30　密度算符的性质

1. 自伴性

$$\hat{\rho}^{\dagger} = \hat{\rho} \tag{1.119}$$

从而若 $\hat{\rho} = \sum_{nm} \rho_{nm} \left|a_n\right\rangle \left\langle a_m\right|$, 则

$$\rho_{nm} = \rho_{mn}^{*} \tag{1.120}$$

若 $\hat{\rho} = \int \mathrm{d}a\mathrm{d}a' \, \rho(a,a') \left|a\right\rangle \left\langle a'\right|$, 则

$$\rho(a,a') = \rho(a',a)^{*} \tag{1.121}$$

2. 闭系统的条件: 若 $\sum_i p_i = 1$ 或 $\int \mathrm{d}\lambda \, f(\lambda) = 1$, 则称系统为闭系统 (closed system), 条件为

$$\mathrm{tr}\,\hat{\rho} = 1 \tag{1.122}$$

3. 纯度 (purity): $\mathrm{tr}\left(\hat{\rho}^2\right) \leq 1$, 当且仅当 $\hat{\rho} = \left|\psi\right\rangle \left\langle\psi\right|$, 即系统为纯态时取等. 对于混合态

$$\mathrm{tr}\left(\hat{\rho}^2\right) < 1 \tag{1.123}$$

1.7　张量积

2 量子动力学

Def. 1 绘景

在描述量子系统的时间演化时, 将时间依赖性如何分配给态矢量和算符, 且保持物理预言不变的约定, 称为绘景 (picture).

2.1 时间演化

2.1.1 时间演化算符

Def. 2 时间演化算符

若双参线性算符 $\hat{U}(t,t_0)$ 满足

1. 幺正性: $\forall t,s\in\mathbb{R}$

$$\hat{U}(t,s)\in \mathrm{U}(\mathscr{H}) \tag{2.1}$$

2. 复合性: $\forall t_2,t_1,t_0\in\mathbb{R}$,

$$\hat{U}(t_2,t_1)\hat{U}(t_1,t_0)=\hat{U}(t_2,t_0) \tag{2.2}$$

3. 连续性: $\forall\,|\psi\rangle\in\mathscr{H}$, $t,s,t_0,s_0\in\mathbb{R}$,

$$\lim_{\substack{t\to t_0\\ s\to s_0}}\left\|\hat{U}(t,s)\,|\psi\rangle-\hat{U}(t_0,s_0)\,|\psi\rangle\right\|=0 \tag{2.3}$$

则称 $\hat{U}(t,t_0)$ 为封闭量子系统的一个时间演化算符 (time evolution operator).

Prop. 1 时间演化算符的性质

1. 单位元

$$\hat{U}(t_0,t_0)=\hat{I} \tag{2.4}$$

2. 逆元

$$\hat{U}(t_0,t)=\hat{U}^{-1}(t,t_0)=\hat{U}^{-1}(t,t_0) \tag{2.5}$$

3. 保持内积: $\forall\,|\psi\rangle\,,|\phi\rangle\in\mathscr{H}$

$$\langle\phi|\hat{U}^{\dagger}(t,t_0)\hat{U}(t,t_0)|\psi\rangle=\langle\phi|\psi\rangle \tag{2.6}$$

Def. 3　态矢量的时间演化

时间演化算符 $\hat{U}(t,t_0)$ 把系统从初始时刻 t_0 的态矢量, 幺正地演化到任意时刻 t 的态矢量.

$$|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle \tag{2.7}$$

Thm. 1　算符的等效演化

要求等效不改变可观测量算符的期望值, 即两种表述给出相同的物理预测, 于是有

$$\hat{A}_{\text{eff}}(t,t_0) = \hat{U}^\dagger(t,t_0)\hat{A}\hat{U}(t,t_0) \tag{2.8}$$

Pf　$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(t_0)|\hat{U}^\dagger(t,t_0)\hat{A}\hat{U}(t,t_0)|\psi(t_0)\rangle = \langle\psi(t_0)|\hat{A}_{\text{eff}(t,t_0)}|\psi(t_0)\rangle$.

Def. 4　跃迁振幅

若系统于初态的归一化态矢量为 $|\psi(t_0)\rangle$, 则对于归一化末态态矢量 $|\psi(t)\rangle$, 定义跃迁振幅 (transition amplitude) 为时间演化算符在指定初末态间的矩阵元

$$\langle\psi(t)|\hat{U}(t,t_0)|\psi(t_0)\rangle \tag{2.9}$$

2.1.2　无穷小时间演化

Def. 5　无穷小时间演化算符, 时间演化生成元, Hamilton 算符

依照一般幺正算符的无穷小变换算符, 定义无穷小时间演化算符 (infinitesimal time evolution operator):

$$\hat{U}(t+\delta t,t) := \hat{I} - \frac{\mathrm{i}}{\hbar}\hat{H}\delta t \tag{2.10}$$

称 $\hat{H}$ 为时间演化生成元 (generator of time evolution), 在量子系统演化过程中, 又称 $\hat{H}$ 为 Hamilton 算符 (Hamiltonian operator).

Rmk　作为时间演化生成元的 Hamilton 算符 $\hat{H} = \hat{H}_{\text{S}}$ 是在 Schröidnger 绘景下的.

Prop. 2　Hamilton 算符的自伴性

Hamilton 算符是一个自伴算符.

$$\hat{H}^\dagger(t) = \hat{H}(t) \tag{2.11}$$

Pf　$\hat{U}^\dagger(t+\delta t,t) = \hat{U}(t-\delta t,t) = \left(\hat{I} - \frac{\mathrm{i}}{\hbar}\hat{H}\delta t\right)^\dagger = \hat{I} + \frac{\mathrm{i}}{\hbar}\hat{H}^\dagger(t)\delta t = \hat{I} + \frac{\mathrm{i}}{\hbar}\hat{H}\delta t$.

2.1.3 时间演化算符的演化方程及其形式解

Thm. 2 时间演化算符的 Schrödinger 方程

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)=\hat{H}\hat{U}(t,t_0) \tag{2.12}$$

Pf $\hat{U}(t+\Delta t,t_0)=\hat{U}(t+\Delta t,t)\hat{U}(t,t_0)=\left(\hat{I}-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t\right)\hat{U}(t,t_0)$,

$\Longrightarrow \hat{U}(t+\Delta t,t_0)-\hat{U}(t,t_0)=-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t\cdot\hat{U}(t,t_0)$,

$\Longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)=\mathrm{i}\hbar\lim\limits_{\Delta t\to 0}\frac{\hat{U}(t+\Delta t,t_0)-\hat{U}(t,t_0)}{\Delta t}=\hat{H}\hat{U}(t,t_0)$.

Thm. 3 Hamilton 算符不含时情形的解

若 Hamilton 算符不含时, 则形式解为

$$\hat{U}(t,t_0)=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)} \tag{2.13}$$

Pf 将 $t-t_0$ 平均分为 N 份. 令 $t_0=t_{(0)}$, $t=t_{(N)}$, $N\to\infty$, 则

$$\hat{U}(t_{(k+1)},t_{(k)})=\hat{I}-\frac{\mathrm{i}}{\hbar}\hat{H}(t_{(k)})\Delta t+O(\Delta t^2)\qquad \hat{U}(t,t_0)=\lim_{N\to\infty}\prod_{k=0}^{N-1}\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}(t_{(k)})\Delta t\right)$$

其中 $\Delta t=t_{(k+1)}-t_{(k)}$. 若 $\hat{H}=\mathrm{Const}$, 则

$$\hat{U}(t,t_0)=\lim_{N\to\infty}\left[\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t\right)\right]^N=\lim_{N\to\infty}\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}N\Delta t\right)=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)}$$

Thm. 4 含时而彼此对易情形的解

若含时 Hamilton 算符于不同时刻对易, 即 $\forall t_1,t_2\in\mathbb{R}$, $\left[\hat{H}(t_1),\hat{H}(t_2)\right]=0$, 则形式解为

$$\hat{U}(t,t_0)=\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,\mathrm{d}t'\right) \tag{2.14}$$

Pf 由 $\left[\hat{H}(t_{(k)}),\hat{H}(t_{(l)})\right]=0$, 有 $\mathrm{e}^{\hat{H}(t_{(k)})}\mathrm{e}^{\hat{H}(t_{(l)})}=\mathrm{e}^{\hat{H}(t_{(k)})+\hat{H}(t_{(l)})}$, 从而

$$\hat{U}(t,t_0)=\lim_{N\to\infty}\prod_{k=0}^{N-1}\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}(t_{(k)})\Delta t\right)=\lim_{N\to\infty}\exp\left[-\frac{\mathrm{i}}{\hbar}\sum_{k=0}^{N-1}\hat{H}(t_{(k)})\Delta t\right]=\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,\mathrm{d}t'\right)$$

Thm. 5　Dyson 级数

若含时 Hamilton 算符于不同时刻不对易, 则形式解为

$$\begin{aligned}\hat{U}(t,t_0) &= \mathcal{T}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,\mathrm{d}t'\right)\\ &:= \hat{I}+\sum_{n=1}^{\infty}\left(-\frac{\mathrm{i}}{\hbar}\right)^{n}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)\end{aligned}\tag{2.15}$$

Rmk　其中 $\mathcal{T}$ 称为时间排序算符 (time-ordering operator), 作用于含时算符, 使其按照时间先后顺序降序排序

$$\mathcal{T}\left\{\hat{A}(t_1)\hat{B}(t_2)\right\}=\begin{cases}\hat{A}(t_1)\hat{B}(t_2) & t_1>t_2\\ \hat{B}(t_2)\hat{A}(t_1) & t_1<t_2\end{cases}\tag{2.16}$$

$\mathcal{T}\exp$ 称为时间排序指数 (time-ordered exponential), 由 Dyson 级数定义.

Pf　对时间演化算符的 Schrödinger 方程在 t_0 到 t 积分

$$\int_{t_0}^{t}\frac{\partial}{\partial t}\hat{U}(t_1,t_0)\,\mathrm{d}t_1=\hat{U}(t,t_0)-\hat{I}=-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t_1\,\hat{H}(t_1)\hat{U}(t_1,t_0)$$

其中 $\hat{U}(t_1,t_0)$ 为 $\hat{U}(t,t_0)=\hat{I}-\dfrac{\mathrm{i}}{\hbar}\displaystyle\int_{t_0}^{t}\mathrm{d}t_1\,\hat{H}(t_1)\hat{U}(t_1,t_0)$ 的比 $\hat{I}$ 高一阶的项. 继续迭代

$$\begin{aligned}\hat{U}(t,t_0) &= \hat{I}-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t_1\,\hat{H}(t_1)\left[\hat{I}-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t_1}\mathrm{d}t_2\,\hat{H}(t_2)\hat{U}(t_2,t_0)\right]\\ &= \hat{I}+\left(-\frac{\mathrm{i}}{\hbar}\right)\int_{t_0}^{t}\mathrm{d}t_1\,\hat{H}(t_1)+\left(-\frac{\mathrm{i}}{\hbar}\right)^{2}\int_{t_0}^{t}\int_{t_0}^{t_1}\mathrm{d}t_2\,\hat{H}(t_1)\hat{H}(t_2)\hat{U}(t_2,t)\end{aligned}$$

迭代 N 次后, 有

$$\begin{aligned}\hat{U}(t,t_0) &= \hat{I}+\sum_{n=1}^{N}\left(-\frac{\mathrm{i}}{\hbar}\right)^{n}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)\hat{U}(t_n,t_0)\\ &= \hat{I}+\sum_{n=1}^{N}\left(-\frac{\mathrm{i}}{\hbar}\right)^{n}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)+\hat{R}_{N+1}(t,t_0)\\ R_{N+1} &= \left(-\frac{\mathrm{i}}{\hbar}\right)^{N+1}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_N}\mathrm{d}t_{N+1}\,\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_{N+1})\hat{U}(t_{N+1},t_0)\end{aligned}$$

迭代无穷多次, 则余项趋于零 $\lim\limits_{N\to\infty}\hat{R}_{N+1}(t,t_0)=0$, 得到 Dyson 级数. 由此得证.

2.1.4 时间平移不变性

Def. 6 时间平移不变性

若对系统整体进行时间平移 τ, 而时间演化不变, 即 $\forall \tau, t_1, t_2 \in \mathbb{R}$,

$$\hat{U}(t+\tau, t_0+\tau) = \hat{U}(t, t_0) \tag{2.17}$$

则称系统具有时间平移不变性.

Prop. 3 时间平移不变性下时间演化算符

系统具有时间平移不变性 $\Longleftrightarrow$ 系统的时间演化算符仅依赖于时间差, 即

$$\hat{U}(t, t_0) = \hat{U}(t - t_0) \tag{2.18}$$

Pf 令 $\tau = -t_0$, $\hat{U}(t-t_0, 0) = \hat{U}(t-t_0) = \hat{U}(t, t_0)$.

Thm. 6 时间平移不变性的判定

系统具有时间平移不变性 $\Longleftrightarrow$ Hamilton 算符不显含时间, 即

$$\frac{\partial \hat{H}}{\partial t} = 0 \tag{2.19}$$

Pf "$\Leftarrow$": 由 $\hat{H}$ 不含时情形 $\hat{U}(t, t_0) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)}$ 可得.
"$\Rightarrow$": $\hat{U}(t+\delta t, t) = \hat{U}(\delta t) = \hat{I} - \dfrac{\mathrm{i}}{\hbar}\hat{H}\delta t$, $\hat{U}(\delta t)$ 不含时, 从而 $\hat{H}$ 一定不含时.

2.2 Schrödinger 绘景

在 Schrödinger 绘景下, 态矢量承担了全部的动力学演化任务, 而可观测量算符在除了显式含时的情况外, 固定不动.

2.2.1 态矢量的动力学演化

Thm. 7 Schrödinger 方程

在 Schrpdinger 绘景下, 态矢量随时间演化. 一个态矢量 $|\psi(t)\rangle$ 的动力学演化, 遵循 Schrödinger 方程

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{2.20}$$

Pf 将时间演化算符的 Schrödinger 方程作用于态矢量.

Prop. 4　Schrödinger 绘景下的物理图像

给定态矢量的初值 $|\psi(0)\rangle$ 与 Hamilton 算符 $\hat{H}$, 则于下一次测量前的量子态的动力学演化可由 Schrödinger 方程唯一决定, 而态矢量给出测量可观测量的概率分布.

$$|\psi(t_0)\rangle \xrightarrow{\text{evolution}} |\psi(t)\rangle \xrightarrow[a\text{-outcome}]{\hat{A}\text{-measurement}} |a\rangle = |\phi(t_0')\rangle \xrightarrow{\text{evolution}} |\phi(t')\rangle \to \cdots$$

Cor. 1　左矢的时间演化

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)| = \langle\psi(t)|\hat{H} \tag{2.21}$$

Pf　对 Schrödinger 方程两边取伴随, 再由 Hamilton 算符的自伴性可得.

2.2.2　Ehrenfest 定理

Prop. 5　Schrp̈dinger 绘景下的可观测量算符

在 Schrp̈dinger 绘景下, 可观测量算符不随时间发生动力学演化, 因此其时间依赖必定来源于显式时间依赖, 即

$$\frac{\mathrm{d}\hat{O}}{\mathrm{d}t} = \frac{\partial\hat{O}}{\partial t} \neq 0 \tag{2.22}$$

若其本身不显含时间 $\dfrac{\partial\hat{F}}{\partial t} = 0$, 则 $\dfrac{\mathrm{d}\hat{F}}{\mathrm{d}t} = 0$, 称为不含时可观测量算符 (time-independent operator).

Thm. 8　Ehrenfest 定理

在 Schrödinger 绘景下, 可观测量算符的期望值满足 Ehrenfest 定理

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{O}\right\rangle(t) = \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle + \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{O},\hat{H}\right]\right\rangle \tag{2.23}$$

Pf　由左右矢的 Schrödinger 方程,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{O}\right\rangle(t) &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\langle\psi(t)|\hat{O}|\psi(t)\rangle\right) = \left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\right)\hat{O}|\psi(t)\rangle + \langle\psi(t)|\frac{\mathrm{d}\hat{O}}{\mathrm{d}t}|\psi(t)\rangle + \langle\psi(t)|\hat{O}\left(\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\right) \\
&= \left(-\frac{1}{\mathrm{i}\hbar}\langle\psi(t)|\hat{H}\right)\hat{O}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{O}}{\partial t}|\psi(t)\rangle + \langle\psi(t)|\hat{O}\left(\frac{1}{\mathrm{i}\hbar}\hat{H}|\psi(t)\rangle\right) \\
&= \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle + \frac{1}{\mathrm{i}\hbar}\underbrace{\langle\psi(t)|\left[\hat{O},\hat{H}\right]|\psi(t)\rangle}_{=\langle[\hat{O},\hat{H}]\rangle}
\end{aligned}$$

Eg. 1　势场中粒子的 Ehrenfest 定理

一维势场 $V(\hat{x})$ 中的粒子的 Hamilton 算符为

$$\hat{H}=\frac{\hat{p}^2}{2m}+V(\hat{x}) \tag{2.24}$$

由对易关系

$$\left[\hat{x},\hat{H}\right]=\frac{[\hat{x},\hat{p}^2]}{2m}=\mathrm{i}\hbar\frac{\hat{p}}{m}\qquad\left[\hat{p},\hat{H}\right]=-\mathrm{i}\hbar V'(\hat{x}) \tag{2.25}$$

得到

$$\frac{\mathrm{d}\langle\hat{x}\rangle}{\mathrm{d}t}=\frac{\langle\hat{p}\rangle}{m}\qquad\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t}=-\langle V'(\hat{x})\rangle \tag{2.26}$$

从而有 1 维势场中粒子的 Ehrenfest 定理

$$m\frac{\mathrm{d}^2\langle\hat{x}\rangle}{\mathrm{d}t^2}=\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t}=-\langle V'(\hat{x})\rangle \tag{2.27}$$

推广到 3 维势场, 有

$$m\frac{\mathrm{d}^2\langle\hat{\boldsymbol{x}}\rangle}{\mathrm{d}t^2}=\frac{\mathrm{d}\langle\hat{\boldsymbol{p}}\rangle}{\mathrm{d}t}=-\langle\nabla V(\hat{\boldsymbol{x}})\rangle \tag{2.28}$$

Rmk　对于自由粒子, $\hat{H}=\dfrac{\hat{p}^2}{2m}$, $\left[\hat{p},\hat{H}\right]=0$, 从而 $\langle\hat{p}\rangle\equiv\langle\hat{p}\rangle_0$, 即动量守恒.

2.2.3　守恒量与好量子数

Def. 7　守恒量

若 $\dfrac{\partial\hat{O}}{\partial t}=0$, 且 $\left[\hat{O},\hat{H}\right]=0$, 则称 $\hat{O}$ 为一个守恒量 (conserved quantity).

Prop. 6

守恒量 $\hat{O}$ 与 $\hat{H}$ 有共同本征态

Def. 8　好量子数

若守恒量 $\hat{O}$ 有本征方程

$$\hat{O}\left|o\right\rangle=o\left|o\right\rangle \tag{2.29}$$

则称 o 为一个好量子数 (good quantum number).

2.2.4 能量-时间不确定性关系

Thm. 9 能量-时间不确定性关系

$$\Delta E \Delta t \geq \frac{\hbar}{2} \tag{2.30}$$

其中 Δt 为特征时间. 对于可观测量 $\hat{A}$, 若满足 $\dfrac{\partial \hat{A}}{\partial t} = 0$, $\left[\hat{A}, \hat{H}\right] = 0$, 则可定义特征时间

$$\Delta t_A = \frac{\Delta A}{\left|\mathrm{d}\left\langle \hat{A} \right\rangle / \mathrm{d}t\right|} \tag{2.31}$$

Rmk 特征时间 Δt 表征系统量子态变化的快慢,

Pf 由 Ehrenfest 定理, $\dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle = \dfrac{1}{\mathrm{i}\hbar}\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle$. $\Delta A \Delta E \geq \dfrac{1}{2}\left|\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle\right| = \dfrac{\hbar}{2}\left|\dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle\right|$.

2.3 Heisenberg 绘景

在 Heisenberg 绘景下, 态矢量固定不动, 可观测量算符随时间演化, 且保持与 Schrödinger 绘景下相同的物理预言.

2.3.1 可观测量算符的动力学演化

Def. 9 Heisenberg 绘景下的态矢量与可观测量算符

- 定义 Heisenberg 绘景下的态矢量固定为 Schrödinger 绘景下态矢量的初始值

$$\left|\psi_{\mathrm{H}}(t_0)\right\rangle = \left|\psi_{\mathrm{S}}(t_0)\right\rangle \tag{2.32}$$

从而 $\left|\psi_{\mathrm{H}}(t_0)\right\rangle$ 不随时间演化

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi_{\mathrm{H}}(t_0)\right\rangle = 0 \tag{2.33}$$

- 定义 Heisenberg 绘景下的可观测量算符为等效演化的算符

$$\hat{A}_{\mathrm{H}}(t) = \hat{U}^{\dagger}(t, t_0)\hat{A}_{\mathrm{S}}(t)\hat{U}(t, t_0) \tag{2.34}$$

而初始时刻两种绘景下的可观测量算符相同

$$\hat{A}_{\mathrm{H}}(t_0) = \hat{A}_{\mathrm{S}}(t_0) \tag{2.35}$$

- “H” 表示该态矢量或可观测量算符在 Heisenberg 绘景下, “S” 表示其在 Schrödinger 绘景下.

Thm. 10　Heisenberg 方程

在 Heisenberg 绘景下, 可观测量算符随时间演化. 一个可观测量算符 $\hat{A}_{\mathrm{H}}$ 的动力学演化, 遵循 Heisenberg 方程

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_{\mathrm{H}}=\left(\frac{\partial\hat{A}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}}+\frac{1}{\mathrm{i}\hbar}\left[\hat{A}_{\mathrm{H}},\hat{H}_{\mathrm{H}}\right] \tag{2.36}$$

Pf　取 $t_0=0$. 由 $\mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)=\hat{H}_{\mathrm{S}}(t)\hat{U}(t)$, $-\mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\hat{U}^{\dagger}(t)=\hat{U}^{\dagger}(t)\hat{H}^{\dagger}(t)$.

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

Cor. 2　保守体系

对于保守体系 $\dfrac{\partial\hat{H}}{\partial t}=0$, 有 $\left[\hat{U},\hat{H}_{\mathrm{S}}\right]=0$, 从而

$$\hat{H}_{\mathrm{H}}=\hat{H}_{\mathrm{S}} \tag{2.37}$$

Pf　$\left[\hat{U},\hat{H}_{\mathrm{S}}\right]=0,\implies\hat{U}\hat{H}_{\mathrm{S}}=\hat{H}_{\mathrm{S}}\hat{U},\implies\hat{H}_{\mathrm{H}}=\hat{U}^{\dagger}\hat{H}_{\mathrm{S}}\hat{U}=\hat{U}^{\dagger}\hat{U}\hat{H}_{\mathrm{S}}=\hat{H}_{\mathrm{S}}$.

Cor. 3　不显含时间的算符的 Heisenberg 方程

对于不显含时间的算符 $\hat{A}_{\mathrm{H}}$, $\dfrac{\partial\hat{A}_{\mathrm{S}}}{\partial t}=0$, 从而

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_{\mathrm{H}}=\frac{1}{\mathrm{i}\hbar}\left[\hat{A}_{\mathrm{H}},\hat{H}_{\mathrm{H}}\right] \tag{2.38}$$

2.4　相互作用绘景

$$\hat{H}=\hat{H}_0+\hat{V} \tag{2.39}$$

2.5　波动力学

Def. 10　波动力学

波动力学 (wave mechanics) 是在 Schrödinger 绘景下, 以波函数表述量子态的量子力学, 一般选取位置表象或动量表象.

2.6 Feynman 路径积分

two QMs

Lagrangian Path Integral vs Hamiltonian Canonical Quantization

2.6.1 路径积分量子化

Post. 1 路径积分量子化

给出系统的位形流形 (configuration manifold) $\mathcal{Q}$. 对于一条可能的路径 $q:[t_0,t]\to\mathcal{Q}$, 系统沿路径 $q(t)$ 从 (t_0,q_0) 演化到 (t,q), 即满足边界条件 $q(t_0)=q_0, q(t)=q$.
由经典 Lagrange 量 $L=L(q,\dot{q},t)$ 定义作用量泛函 (action functional) 为

$$S[q(t)]=\int_{t_0}^{t}L(q,\dot{q},t)\,\mathrm{d}t \tag{2.40}$$

则 $q(t)$ 贡献的路径振幅权重 (path amplitude weight) 为作用量相位因子

$$\exp\left\{\frac{\mathrm{i}}{\hbar}S[q(t)]\right\} \tag{2.41}$$

而传播子为所有可能的路径所贡献的跃迁振幅权重之和, 即路径积分 (path integral):

$$K(q,t;q_0,t_0)=\int_{q_0}^{q}\mathcal{D}[q(t)]\,\exp\left\{\frac{\mathrm{i}}{\hbar}S[q(t)]\right\} \tag{2.42}$$

其中路径积分的泛函积分测度 (functional integral measure) $\mathcal{D}[q(t)]$ 由时间切片极限 (time-slicing limit) 定义

$$\mathcal{D}[q(t)]:=\lim_{N\to\infty}\mathcal{N}_N\mathrm{d}q_{N-1}\mathrm{d}q_{N-2}\cdots\mathrm{d}q_1=\lim_{N\to\infty}\mathcal{N}_N\prod_{n=1}^{N-1}\mathrm{d}q_n \tag{2.43}$$

Rmk 路径积分中的作用量泛函 $S[q]$ 不同于经典作用量 $S[q_{\mathrm{cl}}]$, 后者要求对于满足运动方程的经典路径定义.

2.6.2 传播子

Def. 11 传播子

传播子 (propagator) 定义为时间演化算符在位形表象 $|q\rangle$ 下的矩阵元

$$K(q,q_0;t,t_0)=\langle q|\hat{U}(t,t_0)|q_0\rangle \tag{2.44}$$

又称 $K(q,q_0;t,t_0)$ 为路径积分核 (path integral kernel).

Prop. 7　传播子的初始条件

$$\lim_{t\to t_0} K(q,t;q_0,t_0) = \langle x|x_0\rangle = \delta(x-x_0) \tag{2.45}$$

Prop. 8　传播子的复合性

$$K(q_2,t_2;q_0,t_0) = K(q_2,t_2;q_1,t_1)K(q_1,t_1;q_0,t_0) \tag{2.46}$$

Eg. 2　波动力学的传播子

定义波动力学中的传播子 (propagator) 为

$$K(\boldsymbol{x},t;\boldsymbol{x}_0,t_0) = \langle \boldsymbol{x}|\hat{U}(t,t_0)|\boldsymbol{x}_0\rangle \tag{2.47}$$

从而给定初始时刻波函数 $\psi(\boldsymbol{x}_0,t_0)$, 则波函数的时间演化为

$$\psi(\boldsymbol{x},t) = \int \mathrm{d}^3x_0\, K(\boldsymbol{x},t;\boldsymbol{x}_0,t_0)\psi(\boldsymbol{x}_0,t_0) \tag{2.48}$$

其中时间演化算符为

$$\hat{U}(t,t_0) = \begin{cases} \exp\left[-\dfrac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)\right] & \dfrac{\partial \hat{H}}{\partial t} = 0 \\ \exp\left[-\dfrac{\mathrm{i}}{\hbar}\displaystyle\int_{t_0}^{t}\hat{H}(t')\,\mathrm{d}t'\right] & \dfrac{\partial \hat{H}}{\partial t} \neq 0, \left[\hat{H}(t_1),\hat{H}(t_2)\right] = 0, \forall t_1,t_2 \in \mathbb{R} \\ \mathcal{T}\exp\left[-\dfrac{\mathrm{i}}{\hbar}\displaystyle\int_{t_0}^{t}\hat{H}(t')\,\mathrm{d}t'\right] & \left[\hat{H}(t_1),\hat{H}(t_2)\right] = 0, \forall t_1,t_2 \in \mathbb{R} \end{cases} \tag{2.49}$$

Pf　$\psi(\boldsymbol{x},t) = \langle \boldsymbol{x}|\psi(t)\rangle = \langle \boldsymbol{x}|\hat{U}(t,t_0)|\psi(t_0)\rangle = \displaystyle\int \mathrm{d}^3x_0\, \langle \boldsymbol{x}|\hat{U}(t,t_0)|\boldsymbol{x}_0\rangle \langle \boldsymbol{x}_0|\psi(t_0)\rangle$.

2.6.3　一维保守粒子的路径积分

将 t_0 至 t 均分为 N 段. 令 $t = t_N$, $x_0 = x(t_0), \cdots, x_N = x(t_N)$, $\Delta t = t_{j+1} - t_j$, $j = 0,1,\cdots,N-1$. 则可将传播子分割为

$$\begin{aligned} K(x,t;x_0,t_0) &= \langle x_N|\hat{U}(t_N,t_0)|x_0\rangle \\ &= \langle x_N|\hat{U}(t_N,t_{N-1})\hat{U}(t_{N-1},t_{N-2})\cdots\hat{U}(t_1,t_0)|x_0\rangle \\ &= \int \prod_{i=1}^{N-1}\mathrm{d}x_i\, \langle x_N|\hat{U}(t_N,t_{N-1})|x_{N-1}\rangle\cdots\langle x_1|\hat{U}(t_1,t_0)|x_0\rangle \\ &= \int \prod_{i=1}^{N-1}\mathrm{d}x_i \prod_{j=0}^{N-1} K(x_{j+1},t_{j+1};x_j,t_j) \end{aligned} \tag{2.50}$$

称其中 $K(x_{j+1},t_{j+1};x_j,t_j) = K(x_{j+1},x_j,\Delta t_j)$ 为短时传播子 (short-time propagator).

粒子的 Hamilton 算符为 $\hat{H}=\dfrac{\hat{p}}{2m}+V(\hat{x})$, 从而 $\hat{U}(\Delta t)=\exp\left\{-\dfrac{\mathrm{i}}{\hbar}\left[\dfrac{\hat{p}^2}{2m}+V(\hat{x})\right](t-t_0)\right\}$. 由 BCH 公式 $\mathrm{e}^{\hat{A}+\hat{B}}=\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{A}}\mathrm{e}^{-\frac{1}{2}\left[\hat{A},\hat{B}\right]}$,

$$\hat{A}=-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}\Delta t\sim\Delta t\qquad \hat{B}=-\frac{\mathrm{i}}{\hbar}V(\hat{x})\Delta t\sim\Delta t \tag{2.51}$$

$$\left[\hat{A},\hat{B}\right]=-\frac{\Delta t^2}{2m\hbar^2}\left[\hat{p}^2,V(\hat{x})\right]\sim\Delta t^2 \tag{2.52}$$

忽略二阶小量, 从而短时传播子为

$$\begin{aligned}K(x_{j+1},x_j,\Delta t)&=\langle x_{j+1}|\hat{U}(t_{j+1},t_j)|x_j\rangle=\langle x_{j+1}|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}\Delta t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(\hat{x})\Delta t}|x_j\rangle\\&=\int\mathrm{d}x\int\mathrm{d}p_j\ \langle x_{j+1}|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}\Delta t}|p_j\rangle\langle p_j|x\rangle\ \langle x|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(\hat{x})\Delta t}|x_j\rangle\\&=\int\mathrm{d}p_j\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p_j^2}{2m}\Delta t}\cdot\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_jx_{j+1}}\cdot\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p_jx_j}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(x_j)\Delta t}\\&=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(x_k)\Delta t}\underbrace{\int\frac{\mathrm{d}p_j}{2\pi\hbar}\exp\left\{-\frac{\mathrm{i}\Delta t}{2m\hbar}\left[p_j^2-\frac{2m}{\Delta t}p_j(x_{j+1}-x_j)\right]\right\}}_{=I}\end{aligned} \tag{2.53}$$

Lem. 1　Gauss 积分

$$\int_{-\infty}^{\infty}\mathrm{e}^{-ap^2}\,\mathrm{d}p=\sqrt{\frac{\pi}{\mathrm{i}a}}\quad(a\in\mathbb{R}^+) \tag{2.54}$$

$$\begin{aligned}I&=\exp\left\{\frac{\mathrm{i}\Delta t}{2m\hbar}\left[\frac{m}{\Delta t}(x_{j+1}-x_j)\right]^2\right\}\frac{1}{2\pi\hbar}\int\mathrm{d}p_j\ \exp\left\{-\frac{\mathrm{i}\Delta t}{2m\hbar}\left[p_j-\frac{m}{\Delta t}(x_{j+1}-x_j)\right]^2\right\}\\&=\exp\left[\frac{\mathrm{i}m}{2\hbar}\left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2\Delta t\right]\sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}}\end{aligned} \tag{2.55}$$

$$\begin{aligned}K(x,t;x_0,t_0)&=\underbrace{\lim_{N\to\infty}\left(\frac{m}{2\pi\mathrm{i}\hbar\Delta t}\right)^{\frac{N}{2}}\int\prod_{i=1}^{N}\mathrm{d}x_i}_{\int_{x_0}^{x}\mathcal{D}[x(t)]}\prod_{j=0}^{N-1}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2-V(x_j)\right]\Delta t\right\}\\&=\int_{x_0}^{x}\mathcal{D}[x(t)]\exp\left\{\frac{\mathrm{i}}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\dot{x}(t_j)^2-V(x_j)\right]\Delta t\right\}\\&=\int_{x_0}^{x}\mathcal{D}[x(t)]\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\left[\frac{m}{2}\dot{x}(t)^2-V(x)\right]\mathrm{d}t\right\}\\&=\int_{x_0}^{x}\mathcal{D}[x(t)]\exp\left[\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}L(x,\dot{x},t)\,\mathrm{d}t\right]=\int_{x_0}^{x}\mathcal{D}[x(t)]\exp\left[\frac{\mathrm{i}}{\hbar}S[x(t)]\right]\end{aligned} \tag{2.56}$$

2.7 非纯态系统的时间演化

2.7.1 密度算符的时间演化方程

Thm. 11 von Neumann 方程

$$\frac{\partial \hat{\rho}}{\partial t}+\frac{1}{\mathrm{i}\hbar}\left[\hat{\rho},\hat{H}\right]=0 \tag{2.57}$$

2.8 量子谐振子

2.8.1 湮灭算符与产生算符

Def. 12 湮灭算符与产生算符

引入无量纲位置算符与动量算符

$$\hat{X}=\sqrt{\frac{m\omega}{\hbar}}\hat{x}\qquad \hat{P}=\frac{1}{\sqrt{m\omega\hbar}}\hat{p} \tag{2.58}$$

由此定义湮灭算符 (annihilation operator) 与产生算符 (creation operator)

$$\hat{a}=\frac{1}{\sqrt{2}}\left(\hat{X}+\mathrm{i}\hat{P}\right)=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{\mathrm{i}\hat{p}}{m\omega}\right)=\sqrt{\frac{m\omega}{2\hbar}}\hat{x}+\mathrm{i}\frac{\hat{p}}{\sqrt{2m\hbar\omega}} \tag{2.59}$$

$$\hat{a}^{\dagger}=\frac{1}{\sqrt{2}}\left(\hat{X}-\mathrm{i}\hat{P}\right)=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}-\frac{\mathrm{i}\hat{p}}{m\omega}\right)=\sqrt{\frac{m\omega}{2\hbar}}\hat{x}-\mathrm{i}\frac{\hat{p}}{\sqrt{2m\hbar\omega}} \tag{2.60}$$

湮灭算符 $\hat{a}$ 与产生算符 $\hat{a}^{\dagger}$ 均不是自伴算符.

Prop. 9 量子谐振子的 Hamilton 算符

由正则量子化, 可得量子谐振子 (quantum harmonic oscillator) 的 Hamilton 算符为

$$\hat{H}=\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{x}^2 \tag{2.61}$$

可用湮灭算符与产生算符写为

$$\hat{H}=\hbar\omega\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\hat{I}\right) \tag{2.62}$$

Pf 由无量纲的基本对易关系 $\left[\hat{X},\hat{P}\right]=\frac{1}{\hbar}[\hat{x},\hat{p}]=\mathrm{i}\hat{I}$.

$$\hat{a}^{\dagger}\hat{a}=\frac{1}{2}\left(\hat{X}^2+\mathrm{i}\left[\hat{X},\hat{P}\right]+\hat{P}^2\right)=\frac{1}{2}\left(\frac{m\omega}{\hbar}\hat{x}^2+\frac{\hat{p}^2}{m\hbar\omega}-\hat{I}\right)=\frac{1}{\hbar\omega}\underbrace{\left(\frac{1}{2}m\omega^2\hat{x}^2+\frac{\hat{p}^2}{2m}\right)}_{=\hat{H}_{\mathrm{QHO}}}-\frac{1}{2}\hat{I}$$

Thm. 12　湮灭算符与产生算符的对易关系

$$\left[\hat{a},\hat{a}^\dagger\right]=\hat{I} \tag{2.63}$$

Pf　$\left[\hat{a},\hat{a}^\dagger\right]=\frac{1}{2}\left[\hat{X}+\mathrm{i}\hat{P},\hat{X}-\mathrm{i}\hat{P}\right]=\frac{1}{2}\left(\left[\hat{X},\hat{X}\right]+\mathrm{i}\left[\hat{P},\hat{X}\right]-\mathrm{i}\left[\hat{X},\hat{P}\right]-\mathrm{i}^2\left[\hat{P},\hat{P}\right]\right)=\hat{I}.$

2.8.2　粒子数算符

Def. 13　粒子数算符与 Fock 态

利用 $\hat{a}^\dagger$ 与 $\hat{a}$ 的乘积, 构造出一个自伴算符, 定义为粒子数算符 (number operator):

$$\hat{N}=\hat{a}^\dagger\hat{a} \tag{2.64}$$

粒子数算符的本征方程为

$$\hat{N}\left|n\right\rangle=n\left|n\right\rangle \tag{2.65}$$

称其本征态 $\left|n\right\rangle$ 为数态 (number state), 或称为 Fock 态 (Fock state).

Prop. 10　粒子数算符的对易关系

$$\left[\hat{N},\hat{a}\right]=-\hat{a}\qquad\left[\hat{N},\hat{a}^\dagger\right]=+\hat{a}^\dagger \tag{2.66}$$

Pf　$\left[\hat{N},\hat{a}\right]=\left[\hat{a}^\dagger\hat{a},\hat{a}\right]=\hat{a}^\dagger\underbrace{\left[\hat{a},\hat{a}\right]}_{=0}+\underbrace{\left[\hat{a}^\dagger,\hat{a}\right]}_{=-\hat{I}}\hat{a}=-\hat{a}.$　$\left[\hat{N},\hat{a}^\dagger\right]=\hat{a}^\dagger\left[\hat{a},\hat{a}^\dagger\right]+\left[\hat{a}^\dagger,\hat{a}^\ddagger\right]\hat{a}=\hat{a}^\dagger.$

Prop. 11　湮灭算符与产生算符对 Fock 态的作用

设粒子数算符的本征方程为 $\hat{N}\left|n\right\rangle=n\left|n\right\rangle$, 则有

$$\hat{N}(\hat{a}\left|n\right\rangle)=(n-1)\hat{a}\left|n\right\rangle \tag{2.67}$$

$$\hat{N}(\hat{a}^\dagger\left|n\right\rangle)=(n+1)\hat{a}^\dagger\left|n\right\rangle \tag{2.68}$$

湮灭算符将 n Fock 态下降为 $n-1$ Fock 态, 即湮灭了一个粒子; 产生算符将 n Fock 态上升为 $n+1$ Fock 态, 即产生了一个粒子.
由归一化条件可得

$$\hat{a}\left|n\right\rangle=\sqrt{n}\left|n-1\right\rangle \tag{2.69}$$

$$\hat{a}^\dagger\left|n\right\rangle=\sqrt{n+1}\left|n+1\right\rangle \tag{2.70}$$

Pf　$\hat{N}\hat{a}\left|n\right\rangle=\left[\hat{N},\hat{a}\right]\left|n\right\rangle+\hat{a}\hat{N}\left|n\right\rangle=-\hat{a}\left|n\right\rangle+n\hat{a}\left|n\right\rangle=(n-1)\hat{a}\left|n\right\rangle.$
$\hat{H}\hat{a}^\dagger\left|n\right\rangle=\left[\hat{N},\hat{a}^\dagger\right]\left|n\right\rangle+\hat{a}^\dagger\hat{N}\left|n\right\rangle=\hat{a}^\dagger\left|n\right\rangle+n\hat{a}^\dagger\left|n\right\rangle=(n+1)\hat{a}^\dagger\left|n\right\rangle.$
Assume $\hat{a}\left|n\right\rangle=c\left|n-1\right\rangle$, $c\in\mathbb{R}^+$. Then $\left\langle n|\hat{a}^\dagger\hat{a}|n\right\rangle=\left\langle n|\hat{N}|n\right\rangle=n\left\langle n|n\right\rangle=n=c^2$, $c=\sqrt{n}$.

由 $\left[\hat{a},\hat{a}^\dagger\right]=\hat{I}$, 有 $\hat{a}\hat{a}^\dagger=\hat{N}+\hat{I}$. Assume $\hat{a}^\dagger|n\rangle=d|n+1\rangle$, then $d^2=\langle n|\hat{N}+\hat{I}|n\rangle=n+1$, $d=\sqrt{n+1}$.

Cor. 4　零本征态与 n 的取值

$|0\rangle$ 为湮灭算符 $\hat{a}$ 的本征态, 称为零本征态, 又称为真空态 (vacuum state).

$$\hat{a}|0\rangle=0|0\rangle \tag{2.71}$$

由内积的正定性, 可得 $n\geq 0$. 对 $n>0$ Fock 态不断作用湮灭算符:

$$\begin{aligned}\hat{a}|n\rangle&=\sqrt{n}|n-1\rangle\\ \hat{a}^2|n\rangle&=\sqrt{n(n-1)}|n-2\rangle\\ &\vdots\\ \hat{a}^n|n\rangle&=\sqrt{n!}|0\rangle\\ \hat{a}^{n+1}|n\rangle&=\sqrt{n!}\hat{a}|0\rangle=0|0\rangle\end{aligned} \tag{2.72}$$

从而 n 于 0 处中断. 若 $n\notin\mathbb{N}$, 将不会中断, 导致 $n<0$, 与正定性相悖. 由此 $n\in\mathbb{N}$.

Pf　$\|\hat{a}|0\rangle\|^2=\langle 0|\hat{a}^\dagger\hat{a}|0\rangle=\langle 0|\hat{N}|0\rangle=0,\implies\hat{a}|0\rangle=0|0\rangle$.

Thm. 13　归一化 Fock 态与 Fock 表象

归一化的 n Fock 态的表达式为

$$|n\rangle=\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \tag{2.73}$$

且 $\{|n\rangle\mid n=0,1,2,\cdots\}$ 构成一个完备正交基, 满足

$$\langle m|n\rangle=\delta_{mn}\qquad\sum_{n=0}^{\infty}|n\rangle\langle n|=\hat{I} \tag{2.74}$$

以 Fock 态 $\{|n\rangle\mid n=0,1,2,\cdots\}$ 作为基的表象, 称为 Fock 表象 (Fock representation), 又称为数表象 (number rep), 或占据数表象 (occupation-number rep).

Pf　对 0 Fock 态不断作用产生算符:

$$\begin{cases}\hat{a}^\dagger|0\rangle=|1\rangle\\ \hat{a}^\dagger|1\rangle=\sqrt{2}|2\rangle & \implies|2\rangle=\dfrac{(\hat{a}^\dagger)^2}{\sqrt{2}}\\ \hat{a}^\dagger|2\rangle=\sqrt{3}|3\rangle & \implies|3\rangle=\dfrac{(\hat{a}^\dagger)^3}{\sqrt{3!}}\\ \quad\vdots\\ \hat{a}^\dagger|n-1\rangle=\sqrt{n}|n\rangle & \implies|n\rangle=\dfrac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\end{cases}$$

Prop. 12　湮灭算符与产生算符的矩阵元

$$\langle n'|\hat{a}|n\rangle = \delta_{n',n-1}\sqrt{n} \qquad \langle n'|\hat{a}^\dagger|n\rangle = \delta_{n',n+1}\sqrt{n+1} \tag{2.75}$$

2.8.3　代数求解

Thm. 14　能谱定理

由于 $\left[\hat{N},\hat{H}\right]=0$, 从而可用 $\hat{N}$ 的本征值 $n\in\mathbb{N}$ 标记能量本征态.

$$\hat{H}\,|n\rangle = \hbar\omega\left(\hat{N}+\frac{1}{2}\hat{I}\right)|n\rangle = \left(n+\frac{1}{2}\right)\hbar\omega\,|n\rangle \tag{2.76}$$

从而量子谐振子的能量本征值为

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega \quad (n=0,1,2,\cdots) \tag{2.77}$$

Rmk　此处 $\hat{a}$ 与 $\hat{a}^\dagger$ 湮灭与产生粒子应理解为湮灭或产生一个振动模式的能量量子 $\hbar\omega$.

Cor. 5　零点能

$n=0$ 时, $E_0=\dfrac{1}{2}\hbar\omega$, 称为量子谐振子的零点能 (zero point energy), 或者基态能 (ground state energy).

Rmk　零点能的存在源于 $\hat{a}$ 与 $\hat{a}^\dagger$ 的不对易, 是由量子效应导致的.

Prop. 13　以湮灭算符与产生算符表示位置算符与动量算符

$$\hat{X} = \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger+\hat{a}\right) \qquad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger+\hat{a}\right) \tag{2.78}$$

$$\hat{P} = \frac{\mathrm{i}}{\sqrt{2}}\left(\hat{a}^\dagger-\hat{a}\right) \qquad \hat{p} = \mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}^\dagger-\hat{a}\right) \tag{2.79}$$

Thm. 15　位置算符与动量算符的矩阵元

$$\langle n'|\hat{x}|n\rangle = \frac{\hbar}{2m\omega}\left(\delta_{n',n+1}\sqrt{n+1}+\delta_{n',n-1}\sqrt{n}\right) \tag{2.80}$$

$$\langle n'|\hat{p}|n\rangle = \frac{m\hbar\omega}{2}\left(\delta_{n',n+1}\sqrt{n+1}-\delta_{n',n-1}\sqrt{n}\right) \tag{2.81}$$

Cor. 6　量子谐振子的选择定则

当 $n'=n-1$ 或 $n'=n+1$ 时矩阵元非零, 从而选择定则为

$$\Delta n = \pm 1 \tag{2.82}$$

即量子谐振子与外场线性耦合时, 只能发射或吸收一个能量量子 $\hbar\omega$.

Lem. 2　量子谐振子位置与动量的期望值

$$\langle\hat{x}\rangle = \langle\hat{p}\rangle = 0 \tag{2.83}$$

$$\left\langle\hat{x}^2\right\rangle = \frac{\hbar}{2m\omega}(2n+1) \qquad \left\langle\hat{p}^2\right\rangle = \frac{m\hbar\omega}{2}2n+1 \tag{2.84}$$

Pf　$\hat{x}^2 = \dfrac{\hbar}{2m\omega}\left((\hat{a}^\dagger)^2 + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^2\right) = \dfrac{\hbar}{2m\omega}\left((\hat{a}^\dagger)^2 + \hat{a}^2 + 2\hat{a}^\dagger\hat{a} + \left[\hat{a},\hat{a}^\dagger\right]\right)$.

由于 $\langle n|(\hat{a}^\dagger)^2|n\rangle = \langle n|\hat{a}^2|n\rangle = 0$, $\langle n|2\underbrace{\hat{a}^\dagger\hat{a}}_{=\hat{N}} + \underbrace{\left[\hat{a},\hat{a}^\dagger\right]}_{=\hat{I}}|n\rangle = 2n+1$. 从而 $\left\langle\hat{x}^2\right\rangle = \dfrac{\hbar}{2m\omega}(2n+1)$,

同理有 $\left\langle\hat{p}^2\right\rangle = \dfrac{m\hbar\omega}{2}2n+1$.

Prop. 14　量子谐振子的位置-动量不确定性关系

$$\Delta x\Delta p = \left(n+\frac{1}{2}\right)\hbar \tag{2.85}$$

Pf　$\Delta x^2\Delta p^2 = \left(\left\langle\hat{x}^2\right\rangle - \langle\hat{x}\rangle^2\right)\left(\left\langle\hat{p}^2\right\rangle - \langle\hat{p}\rangle^2\right) = \left\langle\hat{x}^2\right\rangle\left\langle\hat{p}^2\right\rangle = \hbar^2\left(n+\dfrac{1}{2}\right)^2$.

2.8.4　谐振子的时间演化

Prop. 15　湮灭算符与产生算符的时间演化

$$\hat{a}_{\mathrm{H}}(t) = \hat{a}(0)\mathrm{e}^{-\mathrm{i}\omega t} \qquad \hat{a}^\dagger_{\mathrm{H}}(t) = \hat{a}^\dagger(0)\mathrm{e}^{\mathrm{i}\omega t} \tag{2.86}$$

Pf　$\dfrac{\partial\hat{a}_{\mathrm{S}}}{\partial t} = \dfrac{\partial\hat{a}^\dagger_{\mathrm{S}}}{\partial t} = \dfrac{\partial\hat{H}_{\mathrm{S}}}{\partial t} = 0$. $\left[\hat{a}_{\mathrm{H}},\hat{H}\right] = \hbar\omega\left[\hat{a}_{\mathrm{H}},\hat{N}_{\mathrm{H}}\right] = \hbar\omega\hat{a}_{\mathrm{H}}$, $\left[\hat{a}^\dagger_{\mathrm{H}},\hat{H}\right] = -\hbar\omega\hat{a}^\dagger_{\mathrm{H}}$.

$$\frac{\mathrm{d}\hat{a}_{\mathrm{H}}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\left[\hat{a}_{\mathrm{H}},\hat{H}\right] = -\mathrm{i}\omega\hat{a}_{\mathrm{H}}(t) \quad \Longrightarrow \quad \hat{a}_{\mathrm{H}}(t) = \hat{a}(0)\mathrm{e}^{-\mathrm{i}\omega t}$$

$$\frac{\mathrm{d}\hat{a}^\dagger_{\mathrm{H}}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\left[\hat{a}^\dagger_{\mathrm{H}},\hat{H}\right] = \mathrm{i}\omega\hat{a}^\dagger_{\mathrm{H}}(t) \quad \Longrightarrow \quad \hat{a}^\dagger_{\mathrm{H}}(t) = \hat{a}(0)\mathrm{e}^{\mathrm{i}\omega t}$$

Prop. 16　运动方程

Lem. 3　Baker-Hausdorff 引理

$$\mathrm{e}^{\mathrm{i}\lambda\hat{G}}\hat{A}\mathrm{e}^{-\mathrm{i}\lambda\hat{G}} = \hat{A} + \mathrm{i}\lambda\left[\hat{G},\hat{A}\right] + \frac{(\mathrm{i}\lambda)^2}{2}\left[\hat{G},\left[\hat{G},\hat{A}\right]\right] + \cdots \tag{2.87}$$

2.8.5 相干态

Def. 14 相干态

湮灭算符 $\hat{a}$ 的归一化本征态, 称为相干态 (coherent state)

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \quad (\alpha \in \mathbb{C}) \tag{2.88}$$

Rmk $\hat{a} \sim \hat{X} + \mathrm{i}\hat{P}$ 为描述量子谐振子的复振幅的算符, 从而相干态的复振幅 α 是完全确定的的.

Prop. 17 相干态的 Fock 态展开

$$|\alpha\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{2.89}$$

3 对称性

3.1 连续对称性与守恒律

Thm. 1 Stone 定理

设 $\left\{\hat{U}(t) \mid t \in \mathbb{R}\right\}$ 为 Hilbert 空间 $\mathscr{H}$ 上的强连续单参幺正群, 满足 $\forall |\psi\rangle \in \mathscr{H}$

$$\lim_{t\to 0} \left\| \hat{U}(t)\,|\psi\rangle - |\psi\rangle \right\| = 0 \tag{3.1}$$

则

3.2 空间平移与动量

3.2.1 空间平移算符的代数性质

Def. 1 空间平移算符

量子力学中的空间平移, 由空间平移算符 (space translation operator) 描述, 若将位置本征态移动 $\boldsymbol{a}$:

$$\hat{T}(\boldsymbol{a})\,|\boldsymbol{x}\rangle := |\boldsymbol{x}+\boldsymbol{a}\rangle \tag{3.2}$$

Rmk $\langle \boldsymbol{x}|\,\hat{T}(\boldsymbol{a})^{\dagger} = \langle \boldsymbol{x}+\boldsymbol{a}|$.

Thm. 2 Abel 群性质

设所有空间平移算符构成的集合为 $\mathscr{T}(3) := \left\{\hat{T}(\boldsymbol{a}) \mid \boldsymbol{a} \in \mathbb{R}^3\right\}$, 在其中定义乘法

$$\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{b}) = \hat{T}(\boldsymbol{b}+\boldsymbol{a}) \tag{3.3}$$

空间平移算符的乘法满足以下群公理: $\forall \boldsymbol{a},\boldsymbol{b},\boldsymbol{c} \in \mathbb{R}^3$

1. 结合律:
$$\left[\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{b})\right]\hat{T}(\boldsymbol{c}) = \hat{T}(\boldsymbol{a})\left[\hat{T}(\boldsymbol{b})\hat{T}(\boldsymbol{c})\right] \tag{3.4}$$
2. 有单位元:
$$\hat{T}(\boldsymbol{0}) = \hat{I} \tag{3.5}$$
3. 有逆元:
$$\hat{T}(\boldsymbol{a})^{-1} := \hat{T}(-\boldsymbol{a}) \tag{3.6}$$

以及乘法交换律

$$\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{b}) = \hat{T}(\boldsymbol{b})\hat{T}(\boldsymbol{a}) \tag{3.7}$$

从而 $\mathscr{T}(3)$ 构成一个 Abel 群.

Pf 乘法封闭性: $\left[\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{b})\right]|\boldsymbol{x}\rangle = \hat{T}(\boldsymbol{a})|\boldsymbol{x}+\boldsymbol{b}\rangle = |\boldsymbol{x}+\boldsymbol{b}+\boldsymbol{a}\rangle = \hat{T}(\boldsymbol{b}+\boldsymbol{a})|\boldsymbol{x}\rangle$.
结合律: $\left[\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{b})\right]\hat{T}(\boldsymbol{c}) = \hat{T}(\boldsymbol{b}+\boldsymbol{a})\hat{T}(\boldsymbol{c}) = \hat{T}(\boldsymbol{c}+\boldsymbol{b}+\boldsymbol{a}) = \hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{c}+\boldsymbol{b}) = \hat{T}(\boldsymbol{a})\left[\hat{T}(\boldsymbol{b})\hat{T}(\boldsymbol{c})\right]$.
单位元: $\hat{T}(\boldsymbol{0})\hat{T}(\boldsymbol{a}) = \hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{0}) = \hat{T}(\boldsymbol{a})$.
逆元: $\hat{T}(\boldsymbol{a})^{-1}\hat{T}(\boldsymbol{a}) = \hat{T}(-\boldsymbol{a})\hat{T}(\boldsymbol{a}) = \hat{T}(\boldsymbol{a}-\boldsymbol{a}) = \hat{T}(\boldsymbol{0})$. 同理, $\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{a})^{-1} = \hat{T}(\boldsymbol{0})$.
交换律: $\left[\hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{b})\right]|\boldsymbol{x}\rangle = |\boldsymbol{x}+\boldsymbol{b}+\boldsymbol{a}\rangle = |\boldsymbol{x}+\boldsymbol{a}+\boldsymbol{b}\rangle = \left[\hat{T}(\boldsymbol{b})\hat{T}(\boldsymbol{a})\right]|\boldsymbol{x}\rangle$.

Prop. 1 空间平移算符的幺正性

空间平移算符为幺正算符, 即

$$\hat{T}(\boldsymbol{a})^\dagger\hat{T}(\boldsymbol{a}) = \hat{T}(\boldsymbol{a})\hat{T}(\boldsymbol{a})^\dagger = \hat{I} \quad\Longleftrightarrow\quad \hat{T}(\boldsymbol{a})^\dagger = \hat{T}(\boldsymbol{a})^{-1} \tag{3.8}$$

Pf Let $|\psi'\rangle = \hat{T}(\boldsymbol{a})|\psi\rangle$, $|\phi'\rangle = \hat{T}(\boldsymbol{a})|\phi\rangle$, then

$$\begin{aligned}\langle\phi'|\psi'\rangle &= \langle\phi|\hat{T}(\boldsymbol{a})^\dagger\hat{T}(\boldsymbol{a})|\psi\rangle = \langle\phi|\left[\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\right]\hat{T}(\boldsymbol{a})^\dagger\hat{T}(\boldsymbol{a})\left[\int \mathrm{d}^3x'\ |\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\right]|\psi\rangle \\ &= \int \mathrm{d}^3x \int \mathrm{d}^3x' \underbrace{\langle\phi|\boldsymbol{x}\rangle\langle\boldsymbol{x}+\boldsymbol{a}|\boldsymbol{x}'+\boldsymbol{a}\rangle}_{=\delta(\boldsymbol{x}-\boldsymbol{x}')}\langle\boldsymbol{x}|\psi\rangle = \langle\phi|\underbrace{\left(\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\right)}_{=\hat{I}}|\psi\rangle\end{aligned}$$

从而 $\hat{T}(\boldsymbol{a})^\dagger\hat{T}(\boldsymbol{a}) = \hat{I}$, 再由乘法交换律, 得证.

Cor. 1 对左矢的作用

$$\langle\boldsymbol{x}|\hat{T}(\boldsymbol{a}) = \langle\boldsymbol{x}-\boldsymbol{a}| \tag{3.9}$$

Pf $\langle\boldsymbol{x}|\hat{T}(\boldsymbol{a}) = \langle\boldsymbol{x}|\left[\hat{T}(\boldsymbol{a})^{-1}\right]^\dagger = \langle\boldsymbol{x}|\left[\hat{T}(-\boldsymbol{a})\right]^\dagger = \langle\boldsymbol{x}-\boldsymbol{a}|$.

Prop. 2 对波函数的作用

$$\hat{T}(\boldsymbol{a}\psi(\boldsymbol{x}) = \psi(\boldsymbol{x}-\boldsymbol{a}) \tag{3.10}$$

Pf $\hat{T}(\boldsymbol{a})\psi(\boldsymbol{x}) = \langle\boldsymbol{x}|\hat{T}(\boldsymbol{a})|\psi\rangle = \langle\boldsymbol{x}-\boldsymbol{a}|\psi\rangle = \psi(\boldsymbol{x}-\boldsymbol{a})$.

Prop. 3 与位置算符的对易关系

$$\left[\hat{\boldsymbol{x}}, \hat{T}(\boldsymbol{a})\right] = \boldsymbol{a}\hat{T}(\boldsymbol{a}) \tag{3.11}$$

Pf $\left[\hat{\boldsymbol{x}}, \hat{T}(\boldsymbol{a})\right]|\psi\rangle = \left[\hat{\boldsymbol{x}}, \hat{T}(\boldsymbol{a})\right]\left(\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\right)|\psi\rangle = \int \mathrm{d}^3x \left[\hat{\boldsymbol{x}}, \hat{T}(\boldsymbol{a})\right]|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\psi\rangle$.
$\left[\hat{\boldsymbol{x}}, \hat{T}(\boldsymbol{a})\right]|\boldsymbol{x}\rangle = \hat{\boldsymbol{x}}\hat{T}(\boldsymbol{a})|\boldsymbol{x}\rangle - \hat{T}(\boldsymbol{a})\hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \hat{\boldsymbol{x}}|\boldsymbol{x}+\boldsymbol{a}\rangle - \boldsymbol{x}\hat{T}(\boldsymbol{x})|\boldsymbol{x}\rangle = \boldsymbol{a}|\boldsymbol{x}+\boldsymbol{a}\rangle = \boldsymbol{a}\hat{T}(\boldsymbol{a})|\boldsymbol{x}\rangle$.

Prop. 4　位置算符的主动变换

$$\hat{\boldsymbol{x}} \to \hat{\boldsymbol{x}}' = \hat{T}(\boldsymbol{a})\hat{\boldsymbol{x}}\hat{T}(\boldsymbol{a})^\dagger = \hat{\boldsymbol{x}} - \boldsymbol{a}\hat{I} \tag{3.12}$$

Pf　$\left[\hat{\boldsymbol{x}}, \hat{T}(\boldsymbol{a})\right] = \boldsymbol{a}\hat{T}(\boldsymbol{a}),\ \Longrightarrow\ \hat{T}(\boldsymbol{a})\hat{\boldsymbol{x}}\hat{T}(\boldsymbol{a})^\dagger = \left[\hat{\boldsymbol{x}}\hat{T}(\boldsymbol{a}) - \boldsymbol{a}\hat{T}(\boldsymbol{a})\right]\hat{T}(\boldsymbol{a})^\dagger = \hat{\boldsymbol{x}} - \boldsymbol{a}\hat{I}.$

3.2.2　空间平移算符的指数形式及其生成元

Thm. 3　空间平移算符的指数形式

空间平移算符可以写为如下指数形式

$$\hat{T}(\boldsymbol{a}) = \exp\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{a}\cdot\hat{\boldsymbol{p}}\right) \tag{3.13}$$

其生成元 $\hat{\boldsymbol{p}}$ 自伴.

Meth. 1　指数形式的导出

1. 对 $\hat{T}(a)$ Taylor 展开

$$\hat{T}(a) = \hat{T}(0) + a\left.\frac{\mathrm{d}\hat{T}(a)}{\mathrm{d}a}\right|_{a=0} + \cdots \tag{3.14}$$

2. 令 $\hat{p} = \mathrm{i}\hbar\left.\dfrac{\mathrm{d}\hat{T}(a)}{\mathrm{d}a}\right|_{a=0}$, 则

$$\hat{T}(a) = \hat{T}(0) - \frac{\mathrm{i}}{\hbar}a\hat{p} + \cdots \tag{3.15}$$

3. 设 $0 < \epsilon \ll 1$, 有无穷小变换

$$\hat{T}(\epsilon) = \hat{I} - \frac{\mathrm{i}}{\hbar}\epsilon\hat{p} \tag{3.16}$$

4. 由导数的定义

$$\frac{\mathrm{d}\hat{T}(a)}{\mathrm{d}a} = \lim_{\epsilon\to 0}\frac{\hat{T}(a+\epsilon) - \hat{T}(a)}{\epsilon} = \lim_{\epsilon\to 0}\frac{\hat{T}(\epsilon) - \hat{I}}{\epsilon}\hat{T}(a) = -\frac{\mathrm{i}}{\hbar}\hat{p}\hat{T}(a) \tag{3.17}$$

积分得到

$$\hat{T}(a) = \underbrace{\hat{T}(0)}_{=\hat{I}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}a\hat{p}} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}a\hat{p}} \tag{3.18}$$

Rmk　称其中 a 为参数, $\hat{p}$ 为生成元.

$$\hat{T}(\epsilon)^\dagger = \hat{I} + \frac{\mathrm{i}}{\hbar}\epsilon\hat{p}^\dagger \tag{3.19}$$

$$\hat{T}(\epsilon)^\dagger\hat{T}(\epsilon) = \hat{I} + \frac{\mathrm{i}}{\hbar}\epsilon\left(\hat{p}^\dagger - \hat{p}\right) + O(\hat{p}^2) = \hat{I} \tag{3.20}$$

因此 $\hat{p}^\dagger = \hat{p}$, 从而 $\hat{p}$ 是自伴算符.

Def. 2　动量算符

称空间平移算符的生成元 $\hat{\boldsymbol{p}}$ 为动量算符 (momentum operator). $\hat{\boldsymbol{p}}$ 是一个自伴算符, 对应的可观测量为动量 $\boldsymbol{p}$.

3.2.3　无穷小平移算符

Def. 3　无穷小平移算符

以无穷小量 $\delta\boldsymbol{a}$ 为参量的指数形式的空间平移算符 $\hat{T}(\delta\boldsymbol{a}) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\delta\boldsymbol{a}\cdot\hat{\boldsymbol{p}}}$ 展开, 保留至一阶项, 定义其为无穷小平移算符 (infinitesimal translation operator)

$$\hat{T}(\delta\boldsymbol{a}) = \hat{I} - \frac{\mathrm{i}}{\hbar}\delta\boldsymbol{a}\cdot\hat{\boldsymbol{p}} \tag{3.21}$$

Pf　$\hat{T}(\boldsymbol{a}) = \hat{T}(\boldsymbol{0}) + a_i\dfrac{\partial\hat{T}(\boldsymbol{a})}{\partial a_i}\bigg|_{\boldsymbol{a}=\boldsymbol{0}} + \cdots$, $\hat{p}_i := \mathrm{i}\hbar\dfrac{\partial\hat{T}(\boldsymbol{a})}{\partial a_i}\bigg|_{\boldsymbol{a}=\boldsymbol{0}}$.

Cor. 2　无穷小平移算符与位置算符的对易关系

$$\left[\hat{\boldsymbol{x}}, \hat{T}(\delta\boldsymbol{a})\right] = \delta\boldsymbol{a}\hat{I} \tag{3.22}$$

Pf　采用一级近似: $\left[\hat{\boldsymbol{x}}, \hat{T}(\delta\boldsymbol{a})\right]|\boldsymbol{x}\rangle = \delta\boldsymbol{a}\,|\boldsymbol{x}+\delta\boldsymbol{a}\rangle \approxeq \delta\boldsymbol{a}\,|\boldsymbol{x}\rangle$.

Meth. 2　由无穷小平移算符导出基本对易关系

$$\left[\hat{x}_i, \hat{T}(\delta a_j)\right] = \left[\hat{x}_i, \hat{I} - \frac{\mathrm{i}}{\hbar}\delta a_j\hat{p}_j\right] = \underbrace{\left[\hat{x}_i, \hat{I}\right]}_{=0} - \frac{\mathrm{i}}{\hbar}\delta a_j[\hat{x}_i, \hat{p}_j] = \delta a_i\hat{I} = \delta_{ij}\delta a_j\hat{I}$$

$$\Longrightarrow [\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}\hat{I}$$

Prop. 5　$\hat{x}\leftrightarrow\hat{p}$ 表象变换的核函数

$$|\psi\rangle = \int \mathrm{d}x\,\psi(x)\,|x\rangle = \int \mathrm{d}p\,\tilde{\psi}(p)\,|p\rangle,\ \psi(x) = \int \mathrm{d}p\,\tilde{\psi}(p)\psi_p(x),$$

$$\psi_p(x) = \langle x|p\rangle = \frac{1}{(2\pi\hbar)^{\frac{1}{2}}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \tag{3.23}$$

$$\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}} \tag{3.24}$$

Pf 由 $\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = 2\pi\delta(k)$,

$$\frac{\mathrm{d}\psi_p(x)}{\mathrm{d}x} = \lim_{\epsilon\to 0}\frac{\psi_p(x+\epsilon)-\psi_p(x)}{\epsilon} = \lim_{\epsilon\to 0}\frac{\langle x+\epsilon|p\rangle - \langle x|p\rangle}{\epsilon} = \lim_{\epsilon\to 0}\frac{\langle x|\hat{T}(-\epsilon)|p\rangle - \langle x|p\rangle}{\epsilon}$$
$$= \lim_{\epsilon\to 0}\frac{\langle x|\left(\hat{I}+\mathrm{i}\epsilon\hat{p}/\hbar\right)|p\rangle - \langle x|p\rangle}{\epsilon} = \frac{\mathrm{i}}{\hbar}p\psi_p(x) \qquad \Longrightarrow \psi_p(x) = N\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}$$

$$\langle p|p'\rangle = \langle p|\left(\int \mathrm{d}x\ |x\rangle\langle x|\right)|p'\rangle = \int \mathrm{d}x\ \langle p|x\rangle\langle x|p'\rangle = N^2\int \mathrm{d}x\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(p-p')x}$$
$$= N^2 2\pi\hbar\delta(p-p') = \delta(p-p') \qquad \Longrightarrow N = \frac{1}{(2\pi\hbar)^{\frac{1}{2}}}$$

3.2.4 空间平移不变性与动量守恒

空间平移不变应理解为平移运动与时间演化无关, 即

$$\begin{array}{ccccc} |\psi(t_0)\rangle & \xrightarrow{\hat{T}(\boldsymbol{a})} & \hat{T}(\boldsymbol{a})|\psi(t_0)\rangle & \xrightarrow{\hat{U}(t,t_0)} & \hat{U}(t,t_0)\hat{T}(\boldsymbol{a})|\psi(t_0)\rangle \\ & \searrow^{\hat{U}(t,t_0)} & & & \| \\ & & \hat{U}(t,t_0)|\psi(t_0)\rangle & \xrightarrow{\hat{T}(\boldsymbol{a})} & \hat{T}(\boldsymbol{a})\hat{U}(t,t_0)|\psi(t_0)\rangle \end{array}$$

Def. 4 空间平移不变性

若 $\forall \boldsymbol{a}\in\mathbb{R}^3$, 系统的时间演化算符与空间平移算符 $\hat{T}(\boldsymbol{a})$ 对易, 即 $\forall t, t_0\in\mathbb{R}$,

$$\left[\hat{U}(t,t_0),\hat{T}(\boldsymbol{a})\right] = 0 \tag{3.25}$$

则称系统具有空间平移不变性 (space translation invariance).

Rmk 若只对某一方向的矢量 $\lambda\boldsymbol{n}$ 有 $\left[\hat{U}(t,t_0),\hat{T}(\lambda\boldsymbol{n})\right]$, $\forall\lambda\in\mathbb{R}$, 则只能称系统具有沿 n 方向的空间平移不变性.

Prop. 6 空间平移不变性下的 Hamilton 算符

设系统的 Hamilton 算符为 $\hat{H}(t)$, 则系统具有空间平移不变性 $\Longleftrightarrow$ Hamilton 算符与空间平移算符对易, 即 $\forall\boldsymbol{a}\in\mathbb{R}^3$,

$$\left[\hat{H}(t),\hat{T}(\boldsymbol{a})\right] = 0 \tag{3.26}$$

Rmk 对于 n 方向, 则为 $\left[\hat{H}(t),\hat{T}(\lambda\boldsymbol{n})\right]$, $\forall\lambda\in\mathbb{R}$.

Pf $\left[\hat{U}(t+\delta t,t),\hat{T}(\boldsymbol{a})\right] = \left[\hat{I}-\frac{\mathrm{i}}{\hbar}\hat{H}(t)\delta t,\hat{T}(\boldsymbol{a})\right] = -\frac{\mathrm{i}}{\hbar}\delta t\left[\hat{H}(t),\hat{T}(\boldsymbol{a})\right] = 0.$

Thm. 4 动量守恒律

系统不同的空间平移不变性将导致不同的动量守恒律 (momentum conservation law).

若系统具有沿 $\boldsymbol{e}_i$ 方向的空间平移不变性, 则有

$$\left[\hat{H}(t), \hat{p}_i\right] = 0 \tag{3.27}$$

即动量的 i 分量守恒.
若 $\forall \boldsymbol{a} \in \mathbb{R}^3$, 系统均有空间平移不变性, 则有

$$\left[\hat{H}, \hat{\boldsymbol{p}}\right] = 0 \tag{3.28}$$

Pf $\forall \lambda \in \mathbb{R}, \left[\hat{H}(t), \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\lambda \boldsymbol{e}_i \cdot \boldsymbol{p}}\right] = -\dfrac{\mathrm{i}}{\hbar}\lambda\left[\hat{H}(t), \boldsymbol{e}_i \cdot \boldsymbol{p}\right]\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\lambda \boldsymbol{e}_i \cdot \boldsymbol{p}} = 0$. 分别取 $\boldsymbol{a} = a_1\boldsymbol{e}_1, a_2\boldsymbol{e}_2, a_3\boldsymbol{e}_3$, $\forall a_1, a_2, a_3 \in \mathbb{R}$. 则 p_1, p_2, p_3 均守恒, 从而矢量 $\boldsymbol{p} = p_1\boldsymbol{e}_1 + p_2\boldsymbol{e}_2 + p_3\boldsymbol{e}_3$ 守恒.

3.3 空间旋转与角动量

3.3.1 Euclid 空间中的旋转

Lem. 1 3 维旋转 Lie 群

Euclid 空间中的旋转变换构成一个 3 维特殊正交群

$$\mathrm{SO}(3) = \left\{R \in \mathrm{End}(\mathbb{R}^3) \mid R^{\mathrm{T}}R = \hat{I}, \det R = 1\right\} \tag{3.29}$$

SO(3) 在映射复合下构成一个非 Abel Lie 群.
Rmk $\det = -1$ 的正交变换, 称为空间反演变换 Π. 其与恒等变换 I 构成一个 2 元群, $\{P, I\} \cong \mathbb{Z}_2$. 且对于 3 维正交群有

$$\mathrm{O}(3) \cong \mathrm{SO}(3) \times \{P, I\} \tag{3.30}$$

Lem. 2 Euler 旋转定理与轴角表示

对于任意 3 维的空间转动 $R \in \mathrm{SO}(3)$, 均存在某一固定单位轴, 在 R 下保持不变

$$R\boldsymbol{n} = \boldsymbol{n} \tag{3.31}$$

从而 $\forall R \in \mathrm{SO}(3)$ 均可表示为绕某一固定单位轴 $\boldsymbol{n}$ 的转动

$$R(\boldsymbol{n}, \theta) =: R(\boldsymbol{\theta}) \tag{3.32}$$

称这种由一个单位矢量 $\boldsymbol{n}$ 表示转轴, $\theta \in \mathbb{R}$ 表示转角的空间旋转表示方法为轴角表示 (axis-angle representation).

Lem. 3　Euler 角表示

任意一个 3 维旋转 $R \in \mathrm{SO}(3)$ 均可表示为连续绕 3 个坐标轴的转动. 若采取 zyz 约定, 则

$$R(\alpha, \beta, \gamma) := R_z(\alpha) R_y(\beta) R_z(\gamma) \tag{3.33}$$

称这种由三个参数 $\alpha, \beta, \gamma \in \mathbb{R}$ 的表示方法为 Euler 角表示 (Euler angle representation).

Rmk　轴角表示与 Euler 角表示在 $\beta \in (0, \pi)$ 时等价, 均给出 3 个独立参数. 在 $\beta = 0, \pi$ 时出现万向锁 (Gimbal lock) 现象, 从而 Euler 角表示失效.

Lem. 4　无穷小旋转变换构成的 Lie 代数及其生成元

3 维旋转有 Ridrigues 公式

$$R(\boldsymbol{n}, \theta)\boldsymbol{v} = \boldsymbol{v}\cos\theta + (1 - \cos\theta)(\boldsymbol{n} \cdot \boldsymbol{v})\boldsymbol{n} + \sin\theta(\boldsymbol{n} \times \boldsymbol{v}) \tag{3.34}$$

取无穷小角度 $\delta\theta$ 为参数, 则有无穷小旋转变换

$$R(\boldsymbol{n}, \delta\theta)\boldsymbol{v} = \boldsymbol{v} + \delta\theta(\boldsymbol{n} \times \boldsymbol{v}) = (I + \delta\theta \boldsymbol{n} \cdot \boldsymbol{G})\boldsymbol{v} \tag{3.35}$$

无穷小旋转变换 $R(\boldsymbol{n}, \delta\theta)$ 构成 Lie 群 $\mathrm{SO}(3)$ 的 Lie 代数 $\mathfrak{so}(3) = \mathrm{T}_I \mathrm{SO}(3)$. 经指数映射, 可得到有限旋转

$$R(\boldsymbol{n}, \theta) = \mathrm{e}^{\theta \boldsymbol{n} \cdot \boldsymbol{G}} \in \mathrm{SO}(3) \tag{3.36}$$

其中 $\boldsymbol{G} = (G_1, G_2, G_3)$ 称为无穷小旋转变换的生成元, 或 Lie 代数 $\mathfrak{so}(3)$ 的生成元.

$$G_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad G_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad G_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.37}$$

生成元的性质:

- $(G_i)_{jk} = -\varepsilon_{ijk}$;
- $G_i^{\mathrm{T}} = -G_i$;
- $[G_i, G_j] = \varepsilon_{ijk} G_k$.

3.3.2 空间旋转算符的代数性质

Def. 5 空间旋转算符

量子力学中的空间旋转, 由空间旋转算符 (space rotation operator) 描述, 其对态矢量的作用为

$$|\psi'\rangle = \hat{R}(\boldsymbol{\theta})\,|\psi\rangle \tag{3.38}$$

Lem. 5 双覆盖

存在满射 Lie 群同态 $\pi : \mathrm{SU}(2) \twoheadrightarrow \mathrm{SO}(3)$, 满足 $\mathrm{Ker}\,\pi = \{\pm I_2\}$, 从而由群同态基本定理, 有

$$\mathrm{SO}(3) \cong \mathrm{SU}(2)/\{\pm I_2\} \tag{3.39}$$

称 π 为 SU(2) 对 SO(3) 的双覆盖 (double cover).

Thm. 5

由下图可从 Euclid 空间上的空间旋转变换得到 Hilbert 空间上的空间旋转算符

$$\begin{array}{ccc} \mathrm{SU}(2) & \xrightarrow{\ \pi\ } & \mathrm{SO}(3) \\ {\scriptstyle\rho}\downarrow & & \downarrow{\scriptstyle\bar{\rho}} \\ \mathrm{U}(\mathscr{H}) & \longrightarrow & \mathrm{U}(\mathscr{H})/\,\mathrm{U}(1) \end{array}$$

即 SU(2) 为 SO(3) 的双覆盖, 而 $\mathrm{U}(\mathscr{H})$ 为 SU(2) 的幺正表示, $\mathrm{U}(\mathscr{H})/\,\mathrm{U}(1)$ 为 SO(3) 的射影幺正表示.

Rmk 若不考虑自旋, 则 $\mathrm{U}(\mathscr{H})$ 即为 SO(3) 的幺正表示.

Prop. 7 幺正性

要求空间旋转不改变态矢量的内积, 则空间旋转算符为幺正算符

$$\hat{R}^\dagger(\boldsymbol{\theta})\hat{R}(\boldsymbol{\theta}) = \hat{R}(\boldsymbol{\theta})\hat{R}^\dagger(\boldsymbol{\theta}) = \hat{I} \quad\Longleftrightarrow\quad \hat{R}^\dagger(\boldsymbol{\theta}) = \hat{R}^{-1}(\boldsymbol{\theta}) \tag{3.40}$$

Pf $\langle\psi_{\mathrm{R}}|\psi_{\mathrm{R}}\rangle = \langle\psi|\hat{R}^\dagger(\boldsymbol{\theta})\hat{R}(\boldsymbol{\theta})|\psi\rangle = \langle\psi|\psi\rangle, \implies \hat{R}^\dagger(\boldsymbol{\theta})\hat{R}(\boldsymbol{\theta}) = \hat{I}.$

3.3.3 指数形式、无穷小旋转算符与生成元

Thm. 6 空间旋转算符的指数形式

与一般幺正变换一样, 空间旋转算符有如下指数形式

$$\hat{R}(\boldsymbol{\theta}) = \hat{R}(\boldsymbol{n},\theta) = \exp\!\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{\theta}\cdot\hat{\boldsymbol{J}}\right) \tag{3.41}$$

Def. 6　角动量算符

称空间旋转算符 $\hat{R}(\boldsymbol{\theta})$ 的生成元 $\hat{\boldsymbol{J}}$ 为角动量算符 (angular momentum operator). $\hat{\boldsymbol{J}}$ 是一个自伴算符, 对应的可观测量为总角动量 $\boldsymbol{J}$.

Def. 7　无穷小旋转算符, 角动量算符

以绕 $\boldsymbol{n}$ 轴方向转动无穷小角度 $\delta\theta$ 的空间旋转, $\delta\boldsymbol{\theta} = \boldsymbol{n}\delta\theta$, $\delta\theta_i = n_i\delta\theta$ 可定义无穷小旋转算符 (infinitesimal rotation operator)

$$\hat{R}(\delta\boldsymbol{\theta}) = \hat{R}(\boldsymbol{n}, \delta\theta) = \hat{I} - \frac{\mathrm{i}}{\hbar}\delta\boldsymbol{\theta}\cdot\hat{\boldsymbol{J}} \tag{3.42}$$

Pf　$\hat{R}(\delta\boldsymbol{\theta}) = \hat{I} - \delta\theta_i \dfrac{\partial\hat{R}}{\partial\theta_i}\Big|_{\boldsymbol{\theta}=\boldsymbol{0}}$, $\hat{J}_i = \mathrm{i}\hbar\dfrac{\partial\hat{R}}{\partial\theta_i}\Big|_{\theta_i=0}$

Thm. 7　角动量对易关系

$$\left[\hat{J}_i, \hat{J}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{J}_k \tag{3.43}$$

3.3.4　标量、矢量、张量算符

Lem. 6　可观测量算符的幺正共轭变换

若要求在空间旋转变换前后给出相同的物理预测, 即可观测量算符的期望值不变, 则可观测量算符需进行幺正共轭变换

$$\hat{A}' = \hat{R}\hat{A}\hat{R}^\dagger \tag{3.44}$$

Pf　$\langle\psi'|\hat{A}'|\psi'\rangle = \langle\psi|\hat{R}^\dagger\hat{A}\hat{R}|\psi\rangle = \langle\psi|\hat{A}|\psi\rangle$, $\Longrightarrow$ $\hat{A} = \hat{R}^\dagger\hat{A}\hat{R}$.

Def. 8　标量算符

在空间旋转算符的作用下不变的算符, 称为标量算符 (scalar operator). 满足

$$\left[\hat{\boldsymbol{J}}, \hat{s}\right] \tag{3.45}$$

3.4 空间反演与宇称

3.4.1 宇称算符

Def. 9 宇称算符

量子力学中的空间反演 (space inversion), 由宇称算符 (parity operator) 描述:

$$\hat{\Pi}\left|\boldsymbol{x}\right\rangle = \left|-\boldsymbol{x}\right\rangle \tag{3.46}$$

Prop. 8 宇称算符的性质

宇称算符自伴、幺正且对合, 即

$$\hat{\Pi}^\dagger = \hat{\Pi}^{-1} = \hat{\Pi} \qquad \hat{\Pi}^2 = \hat{I} \tag{3.47}$$

三性合一, 从而其本征值 $\pi \in \{\pm 1\}$.

Pf $\hat{\Pi}^2\left|\boldsymbol{x}\right\rangle = \hat{\Pi}\left|-\boldsymbol{x}\right\rangle = \left|\boldsymbol{x}\right\rangle$. $\forall \left|\psi\right\rangle \in \mathscr{H}$, $\hat{\Pi}^2\left|\psi\right\rangle = \displaystyle\int \mathrm{d}^3x\ \left\langle\boldsymbol{x}\right|\left.\psi\right\rangle \underbrace{\hat{\Pi}^2\left|\boldsymbol{x}\right\rangle}_{=\left|\boldsymbol{x}\right\rangle} = \left|\psi\right\rangle$.

Def. 10 奇偶宇称

称宇称算符 $\hat{\Pi}$ 的本征值 $\pi \in \{\pm 1\}$ 为宇称 (parity). 称 $\pi_+ = 1$ 为偶宇称 (even parity), 称 $\pi_- = -1$ 为奇宇称 (odd parity).

Cor. 3 动量本征态的宇称

$$\hat{\Pi}\left|\boldsymbol{p}\right\rangle = \left|-\boldsymbol{p}\right\rangle \tag{3.48}$$

3.4.2 奇偶宇称态

Def. 11 奇偶宇称态

宇称算符 $\hat{\Pi}$ 的属于本征值 $\pi = 1$ 的本征态, 称为偶宇称态 (even parity state); 属于 $\pi = -1$ 的本征态, 称为奇宇称态 (odd parity state).

$$\hat{\Pi}\left|\psi_+\right\rangle = \left|\psi_+\right\rangle \qquad \hat{\Pi}\left|\psi_-\right\rangle = -\left|\psi_-\right\rangle \tag{3.49}$$

Prop. 9 位置表象下的波函数

奇偶宇称态的波函数是奇偶函数, 即

$$\psi_+(-\boldsymbol{x}) = \psi_+(\boldsymbol{x}) \qquad \psi_-(-\boldsymbol{x}) = -\psi_-(\boldsymbol{x}) \tag{3.50}$$

Pf $\langle \boldsymbol{x}|\hat{\Pi}|\psi_+\rangle = \begin{cases} \langle -\boldsymbol{x}|\psi_+\rangle = \psi_+(-\boldsymbol{x}) \\ \langle \boldsymbol{x}|\psi_+\rangle = \psi_+(\boldsymbol{x}) \end{cases} \Longrightarrow \psi_+(-\boldsymbol{x}) = \psi_+(\boldsymbol{x}).$

$\langle \boldsymbol{x}|\hat{\Pi}|\psi_-\rangle = \begin{cases} \langle -\boldsymbol{x}|\psi_-\rangle = \psi_-(-\boldsymbol{x}) \\ -\langle \boldsymbol{x}|\psi_-\rangle = -\psi_-(\boldsymbol{x}) \end{cases} \Longrightarrow \psi_-(-\boldsymbol{x}) = -\psi_-(\boldsymbol{x}).$

Def. 12 奇偶宇称空间

偶宇称 $\pi_+ = 1$ 的本征子空间

$$\mathscr{H}_+ := \{|\pi_+\rangle \in \mathscr{H} \mid \Pi\,|\pi_+\rangle = |\pi_+\rangle\} \tag{3.51}$$

称为偶宇称子空间 (even parity subspace).
奇宇称 $\pi_- = -1$ 的本征子空间

$$\mathscr{H}_- := \{|\pi_-\rangle \in \mathscr{H} \mid \Pi\,|\pi_-\rangle = -|\pi_-\rangle\} \tag{3.52}$$

称为奇宇称子空间 (odd parity subspace).

Thm. 8

整个 Hilbert 空间可正交分解为偶宇称子空间与奇宇称子空间的直和.

$$\mathscr{H} = \mathscr{H}_+ \oplus \mathscr{H}_- \tag{3.53}$$

Pf 由宇称算符 $\hat{\Pi}$ 的自伴性可得.

3.4.3 奇偶投影算符

Def. 13 奇偶投影算符

偶投影算符 (even projection operator) $\hat{P}_+$ 与奇投影算符 (odd projection operator) $\hat{P}_-$ 定义为

$$\hat{P}_\pm = \frac{1}{2}\left(\hat{I} \pm \hat{\Pi}\right) \tag{3.54}$$

其满足幂等性 $\hat{P}_\pm^2 = \hat{P}_\pm$ 与自伴性 $\hat{P}_\pm^\dagger = \hat{P}_\pm$, 从而是正交投影算符.

Pf $\hat{P}_\pm^2 = \frac{1}{4}\left(\hat{I} \pm 2\hat{\Pi} + \hat{\Pi}^2\right) = \frac{1}{4}\left(2\hat{I} \pm 2\hat{\Pi}\right) = \hat{P}_\pm.$

$\hat{P}_\pm^\dagger = \frac{1}{2}\left(\hat{I} \pm \hat{\Pi}\right)^\dagger = \frac{1}{2}\left(\hat{I} \pm \hat{\Pi}^\dagger\right) = \hat{P}_\pm.$

Prop. 10　奇偶投影算符的性质

- 完备性

$$\hat{P}_+ + \hat{P}_- = \hat{I} \tag{3.55}$$

- 正交性

$$\hat{P}_+\hat{P}_- = \hat{P}_-\hat{P}_+ = 0 \tag{3.56}$$

- 与宇称算符的对易性

$$\left[\hat{P}_\pm, \hat{\Pi}\right] = 0 \tag{3.57}$$

Pf　$\hat{P}_+ + \hat{P}_- = \frac{1}{2}\left(\hat{I} + \hat{\Pi}\right) + \frac{1}{2}\left(\hat{I} - \hat{\Pi}\right) = \hat{I}$.

Prop. 11　奇偶投影

宇称算符 $\hat{\Pi}$ 有本征方程

$$\hat{\Pi}\left(\hat{P}_\pm |\psi\rangle\right) = \pm\hat{P}_\pm |\psi\rangle \tag{3.58}$$

从而 $\hat{P}_\pm |\psi\rangle$ 为 $\hat{\Pi}$ 的属于本征值 ±1 的本征态.
奇偶投影算符可将任意态 $|\psi\rangle$ 变换为奇偶宇称态

$$\hat{P}_\pm |\psi\rangle = |\psi_\pm\rangle \tag{3.59}$$

Prop. 12　态矢量的奇偶分解

$\forall |\psi\rangle \in \mathscr{H}$, 有唯一的奇偶正交分解

$$|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle \tag{3.60}$$

其中 $|\psi_+\rangle \in \mathscr{H}_+$, $|\psi_-\rangle \in \mathscr{H}_-$. 且有

$$\langle\psi_+|\psi_-\rangle = 0 \tag{3.61}$$

Pf　$|\psi\rangle = \hat{P}_+ |\psi\rangle + \left(\hat{I} - \hat{P}_+\right)|\psi\rangle = \underbrace{\hat{P}_+ |\psi\rangle}_{=|\psi_+\rangle} + \underbrace{\hat{P}_- |\psi\rangle}_{=|\psi_-\rangle}$.

3.4.4　奇偶算符

Def. 14　偶算符

若算符 $\hat{A}_+$ 与宇称算符 $\hat{\Pi}$ 对易, 即满足

$$\left[\hat{\Pi}, \hat{A}_+\right] = 0 \tag{3.62}$$

则称 $\hat{A}_+$ 为一个偶算符 (even operator).

Prop. 13　偶算符的宇称性质

偶算符在宇称变换下不变.

$$\hat{A}_+ = \hat{\Pi}\hat{A}_+\hat{\Pi}^\dagger \tag{3.63}$$

Pf　$\left[\hat{\Pi}, \hat{A}_+\right] = 0, \implies \hat{\Pi}\hat{A}_+ = \hat{A}_+\hat{\Pi}, \implies \hat{A}_+ = \hat{\Pi}\hat{A}_+\hat{\Pi}^\dagger.$

Def. 15　奇算符

若算符 $\hat{A}_-$ 与宇称算符 $\hat{\Pi}$ 反对易, 即满足

$$\left\{\hat{\Pi}, \hat{A}_-\right\} = 0 \tag{3.64}$$

则称 $\hat{A}_-$ 为一个奇算符 (odd operator).

Prop. 14　奇算符的宇称性质

奇算符在宇称变换下符号相反.

$$\hat{A}_- = -\hat{\Pi}\hat{A}_-\hat{\Pi}^\dagger \tag{3.65}$$

Pf　$\left\{\hat{\Pi}, \hat{A}_-\right\} = 0, \implies \hat{\Pi}\hat{A}_- = -\hat{A}_-\hat{\Pi}. \implies \hat{A}_- = -\hat{\Pi}\hat{A}_-\hat{\Pi}^\dagger.$

Thm. 9　算符的奇偶分解

若 $\hat{\Pi}\hat{A}\hat{\Pi}^\dagger = \eta_A\hat{A}$, 其中 $\eta_A \in \{\pm 1\}$, 则称 $\hat{A}$ 有确定宇称. 而一般算符不具有确定宇称.
任意算符均可以分解为偶算符与奇算符之和 $\hat{A} = \hat{A}_+ + \hat{A}_-$.

$$\hat{A}_+ = \frac{1}{2}\left(\hat{A} + \hat{\Pi}\hat{A}\hat{\Pi}^\dagger\right) \qquad \hat{A}_- = \frac{1}{2}\left(\hat{A} - \hat{\Pi}\hat{A}\hat{\Pi}^\dagger\right) \tag{3.66}$$

Thm. 10　奇偶算符的乘法运算

设 $\hat{A}_+, \hat{B}_+$ 与 $\hat{A}_-, \hat{B}_-$ 为任意偶算符与奇算符, 则

算符乘积	奇偶性
$\hat{A}_+\hat{B}_+$	偶算符
$\hat{A}_+\hat{B}_-$	奇算符
$\hat{A}_-\hat{B}_+$	奇算符
$\hat{A}_-\hat{B}_-$	偶算符

Pf　Let $\pi, \pi' \in \{\pm 1\}$, then $\hat{\Pi}\hat{A}_\pi\hat{\Pi}^\dagger = \pi\hat{A}_\pi$ and $\hat{\Pi}\hat{B}_{\pi'}\hat{\Pi}^\dagger = \pi'\hat{B}_{\pi'}$.

$$\hat{\Pi}\hat{A}_\pi\hat{B}_{\pi'}\hat{\Pi}^\dagger = \hat{\Pi}\hat{A}_\pi\hat{\Pi}^\dagger\hat{\Pi}\hat{B}_{\pi'}\hat{\Pi}^\dagger = \pi\pi'\hat{A}_\pi\hat{B}_{\pi'}$$

Prop. 15　对易子与反对易子的宇称性质

设 $\pi,\pi'\in\{\pm1\}$, 则 $\left[\hat{A}_\pi,\hat{B}_{\pi'}\right]$ 与 $\left\{\hat{A}_\pi,\hat{B}_{\pi'}\right\}$ 的宇称均为 $\pi\pi'$. 有

$$\hat{\Pi}\left[\hat{A}_\pi,\hat{B}_{\pi'}\right]\hat{\Pi}^\dagger=\pi\pi'\left[\hat{A}_\pi,\hat{B}_{\pi'}\right]\qquad\hat{\Pi}\left\{\hat{A}_\pi,\hat{B}_{\pi'}\right\}\hat{\Pi}^\dagger=\pi\pi'\left\{\hat{A}_\pi,\hat{B}_{\pi'}\right\}\tag{3.67}$$

Prop. 16　算符函数的宇称性质

若 $f(\hat{A})=\sum_n f_n\hat{A}^n$, 则

- $f(\hat{A}_+)$ 为偶算符;
- 当 $f(\hat{A})$ 为偶函数时, $f(\hat{A}_-)$ 为偶算符; $f(\hat{A})$ 为奇函数时, $f(\hat{A}_-)$ 为奇算符.

Pf　$\hat{\Pi}f(\hat{A}_+)\hat{\Pi}^\dagger=\sum_n f_n\hat{\Pi}\hat{A}_+^n\hat{\Pi}^\dagger=\sum_n f_n\underbrace{\left(\hat{\Pi}\hat{A}_+^n\hat{\Pi}^\dagger\right)\cdots\left(\hat{\Pi}\hat{A}_+^n\hat{\Pi}^\dagger\right)}_{n}=\sum_n f_n\hat{A}^n=f(\hat{A}_+)$.

$\hat{\Pi}f(\hat{A}_-)\hat{\Pi}^\dagger=\sum_n f_n\hat{\Pi}\hat{A}_-^n\hat{\Pi}^\dagger=\sum_n(-1)^n f_n\hat{A}_-^n\neq f(\hat{A}_-)$.

If $f(\hat{A})$ even, $\hat{\Pi}f(\hat{A}_-)\hat{\Pi}^\dagger=\sum_n f_n\hat{A}_-^n=f(\hat{A}_-)$, then $f(\hat{A}_-)$ even.

If $f(\hat{A})$ odd, $\hat{\Pi}f(\hat{A}_-)\hat{\Pi}^\dagger=-\sum_n f_n\hat{A}_-^n=-f(\hat{A}_-)$, then $f(\hat{A}_-)$ odd.

Prop. 17　宇称的保持与翻转 *

偶算符保持宇称, 奇算符翻转宇称.

Eg. 1　$\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{p}}$, $\hat{\boldsymbol{L}}$ 的奇偶性

位置算符与动量算符均为奇算符.

$$\hat{\Pi}\hat{\boldsymbol{x}}\hat{\Pi}^\dagger=-\hat{\boldsymbol{x}}\tag{3.68}$$

$$\hat{\Pi}\hat{\boldsymbol{p}}\hat{\Pi}^\dagger=-\hat{\boldsymbol{p}}\tag{3.69}$$

轨道角动量算符为偶算符

$$\hat{\Pi}\hat{\boldsymbol{L}}\hat{\Pi}^\dagger=\hat{\boldsymbol{L}}\tag{3.70}$$

Pf　$\hat{\Pi}\hat{L}_i\hat{\Pi}^\dagger=\hat{\Pi}\varepsilon_{ijk}\hat{x}_j\hat{p}_k\hat{\Pi}^\dagger=\varepsilon_{ijk}\hat{\Pi}\hat{x}_j\hat{\Pi}^\dagger\hat{\Pi}\hat{p}_k\hat{\Pi}^\dagger=\varepsilon_{ijk}(-\hat{x}_j)(-\hat{p}_k)=\hat{L}_i$.

Def. 16　极矢量与轴矢量

- 满足 $\left\{\hat{\Pi},\hat{v}_i\right\}=0$, 或 $\hat{\Pi}\hat{v}_i\hat{\Pi}^\dagger=-\hat{v}_i$ 的矢量算符, 即奇矢量算符, 对应的矢量 $\boldsymbol{v}$ 称为极矢量 (polar vector), 或称真矢量 (true vector).
- 满足 $\left[\hat{\Pi},\hat{v}_i\right]=0$, 或 $\hat{\Pi}\hat{v}_i\hat{\Pi}^\dagger=\hat{v}_i$ 的矢量算符, 即偶矢量算符, 对应的矢量 $\boldsymbol{v}$ 称为轴矢量 (axial vector), 或称赝矢量 (pseudo vector).

Def. 17　真标量与赝标量

- 奇标量算符 $\hat{Q}$ 对应的标量 Q 称为标量, 或者真标量 (true scalar).
- 偶标量算符 $\hat{Q}$ 对应的矢量 Q 称为赝标量 (pseudo scalar).

3.4.5　与宇称相关的跃迁

Thm. 11　宇称选择定则

设跃迁算符 $\hat{A}$ 有确定宇称 η_A, 初态 $|i\rangle$ 与末态 $|f\rangle$ 的宇称分别为 π_i, π_f. 则要求

$$\pi_f \eta_A \pi_i = 1 \tag{3.71}$$

- 对于偶算符 $\hat{A}_+$, 要求 $\pi_f \pi_i = 1$, 即相同宇称的态允许, 相反宇称的态禁戒.
- 对于奇算符 $\hat{A}_-$, 要求 $\pi_f \pi_i = -1$, 即相反宇称的态允许, 相同宇称的态禁戒.

称该与宇称相关的跃迁规则为宇称选择定则 (parity selection rule), 跃迁能否发生, 还需结合其他选择定则.

Pf　$\langle f|\hat{A}|i\rangle = \langle f|\hat{\Pi}^\dagger \underbrace{\hat{\Pi}\hat{A}\hat{\Pi}^\dagger}_{=\eta_A \hat{A}} \hat{\Pi}|i\rangle = \pi_f \eta_A \pi_i \langle f|\hat{A}|i\rangle, \implies \pi_f \eta_A \pi_i = 1.$

Eg. 2　电偶极跃迁

电偶极矩算符为

$$\hat{\boldsymbol{d}} = \sum_n q_n \hat{\boldsymbol{x}}_n \tag{3.72}$$

由于 $\hat{\boldsymbol{x}}_n$ 为极矢量算符, 故 $\hat{\boldsymbol{d}}$ 为奇算符, 因此电偶极跃迁要求 $\pi_f = -\pi_i$, 即初末态宇称相反.

Eg. 3　磁偶极跃迁

磁偶极矩算符为

$$\hat{\boldsymbol{\mu}} = -\mu_{\mathrm{B}} \sum_n \left(\hat{\boldsymbol{L}}_n + g_s \hat{\boldsymbol{S}}_n\right) \tag{3.73}$$

由于 $\hat{\boldsymbol{L}}_n, \hat{\boldsymbol{S}}_n$ 均为轴矢量算符, 故 $\hat{\boldsymbol{\mu}}$ 为偶算符, 因此磁偶极跃迁要求 $\pi_f = \pi_i$, 即初末宇称相同.

3.5 时间反演

3.5.1 反幺正算符

Def. 18 反线性算符

定义算符 $\hat{\Theta}:\mathscr{H}\to\mathscr{H}$, 若满足 $\forall|\psi\rangle,|\phi\rangle\in\mathscr{H}$, $a,b\in\mathbb{C}$,

$$\hat{\Theta}(a|\psi\rangle,b|\phi\rangle)=a^*\left(\hat{\Theta}|\psi\rangle\right)+b^*\hat{\Theta}|\phi\rangle \tag{3.74}$$

则称 $\hat{\Theta}$ 为一个反线性算符 (anti-linear operator).

Prop. 18 幺正-反幺正算符的乘法规则

设 $\hat{U},\hat{U}_1,\hat{U}_2$ 均为幺正算符, $\hat{\Theta},\hat{\Theta}_1,\hat{\Theta}_2$ 均为反幺正算符.

- $\hat{U}_1\hat{U}_2$ 为幺正算符.
- $\hat{U}\hat{\Theta}$ 为反幺正算符.
- $\hat{\Theta}\hat{U}$ 为反幺正算符.
- $\hat{\Theta}_1\hat{\Theta}_2$ 为幺正算符.

4 相对论量子动力学方程

自然单位制 (natural units, NU)

$$c = \hbar = 1$$

4.1 Klein-Gordon 方程

Thm. 1 自由 Klein-Gordon 方程

$$\left(\partial_\mu \partial^\mu + m^2\right) \phi(t, \boldsymbol{x}) = 0 \tag{4.1}$$

Pf 由自由粒子的相对论色散关系直接正则量子化

$$E^2 - p^2 - m^2 \to \left[\left(\mathrm{i}\frac{\partial}{\partial t}\right)^2 - (-\mathrm{i}\nabla)^2 - m^2\right] \phi(t, \boldsymbol{x}) = -\left[\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2\right] \phi(t, \boldsymbol{x}) = 0$$

定义 d'Alembert 算符

$$\partial_\mu \partial^\mu = \eta_{\mu\nu} \partial^\mu \partial^\nu = \frac{\partial^2}{\partial t^2} - \nabla^2 \tag{4.2}$$

于是可得 Klein-Gordon 方程.

Prop. 1 平面波解与正负能量

取平面波形式的解

$$\phi(t, \boldsymbol{x}) = N \mathrm{e}^{-\mathrm{i}(Et - \boldsymbol{p}\cdot\boldsymbol{x})} = N \mathrm{e}^{-\mathrm{i}p^\mu x_\mu} \tag{4.3}$$

可回到 $E^2 = p^2 + m^2$, 但能量存在正负解

$$E_\pm = \pm\sqrt{p^2 + m^2} \tag{4.4}$$

Prop. 2 4-概率流

参照波动力学的 3-概率流 $\boldsymbol{J}(\boldsymbol{x}, t) = -\dfrac{\mathrm{i}}{2m}\left(\psi^* \nabla\psi - \psi \nabla\psi^*\right)$, 可写出 4-概率流

$$J^\mu = \frac{\mathrm{i}}{2m}\left(\phi^* \partial^\mu \phi - \phi \partial^\mu \phi^*\right) \tag{4.5}$$

满足概率流守恒方程

$$\partial_\mu J^\mu = 0 \tag{4.6}$$

而概率密度为

$$\rho(t, \boldsymbol{x}) = J^0(t, \boldsymbol{x}) = \frac{\mathrm{i}}{2m}\left(\phi^* \frac{\partial \phi}{\partial t} - \frac{\partial \phi^*}{\partial t}\phi\right) \tag{4.7}$$

Thm. 2　电磁 Klein-Gordon 方程

设电磁协变导数为

$$\mathrm{D}_\mu = \partial_\mu + eA_\mu \tag{4.8}$$

则带电 e 的自由粒子的 Klein-Gordon 方程为

$$\left(\mathrm{D}_\mu \mathrm{D}^\mu + m^2\right)\phi = 0 \tag{4.9}$$

带电 e 的自由粒子在电磁场中的相对论色散关系为

$$(H - e\Phi)^2 - (\boldsymbol{p} - e\boldsymbol{A})^2 - m^2 = 0 \tag{4.10}$$

$$\Upsilon(t, \boldsymbol{x})$$

4.2　Dirac 方程

4.2.1　Dirac Hamilton 算符

Post. 1　Dirac Hamilton 算符

设相对论性的 Hamilton 算符对动量是“线性” 的, 具有以下形式

$$\hat{H} = \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} + \beta m \hat{I} \tag{4.11}$$

其中系数 $\beta, \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ 均为互不对易的常矩阵, 且均与 $\hat{p}_i$ 对易. 称 β, α_i 为 Dirac β 矩阵与 Dirac α 矩阵, $i = 1, 2, 3$.

Prop. 3　相对论色散关系对 Dirac 矩阵的约束

若 $\hat{H}$ 满足相对论色散关系 $\hat{H}^2 = \hat{\boldsymbol{p}}^2 + m^2\hat{I}$, 则要求 Dirac 矩阵满足

$$\beta^2 = I \qquad \{\alpha_i, \beta\} = 0 \qquad \{\alpha_i, \alpha_j\} = 2\delta_{ij} I \tag{4.12}$$

Pf　$\hat{H}^2 = \left(\alpha_i \hat{p}_i + \beta m \hat{I}\right)\left(\alpha_j \hat{p}_j + \beta m \hat{I}\right) = \alpha_i\alpha_j\hat{p}_i\hat{p}_j + m\{\alpha_i, \beta\}\hat{p}_i + \beta^2 m^2 \hat{I} = \hat{p}_i\hat{p}_i + m^2\hat{I}$. 从而 $\beta^2 = I$, $\{\alpha_i, \beta\} = I$. $\alpha_i\alpha_j\hat{p}_i\hat{p}_j = \dfrac{1}{2}(\alpha_i\alpha_j\hat{p}_i\hat{p}_j + \alpha_i\alpha_j\hat{p}_j\hat{p}_i) = \underbrace{\dfrac{1}{2}[\alpha_i, \alpha_j]}_{=\delta_{ij}I}\hat{p}_i\hat{p}_j = \hat{p}_i\hat{p}_i$.

Prop. 4　Dirac 矩阵的性质

- 三性合一: 自伴、幺正、对合.
- 本征值为 ± 1.

- 均为无迹矩阵, 即

$$\operatorname{tr}\beta = \operatorname{tr}\alpha_i = 0 \tag{4.13}$$

- 必为偶数阶矩阵.

Pf 由 $\hat{H}^\dagger = \hat{H}$ 可得自伴性. 由 $\beta^2 = I$, $\{\alpha_i, \alpha_i\} = 2\alpha_i^2 = 2I$ 可得对合性. 从而幺正, 本征值必为 ± 1. 由 $\{\alpha_i, \beta\} = 0$, $\alpha_i = -\beta\alpha_i\beta$, $\operatorname{tr}\alpha_i = -\operatorname{tr}(\beta\alpha_i\beta) = -\operatorname{tr}(\alpha_i\beta^2) = -\operatorname{tr}\alpha_i$, 从而 $\operatorname{tr}\alpha_i = 0$, 同理 $\operatorname{tr}\beta = 0$. 由于迹为本征值之和, 本征值必须 ± 1 成对出现, 因此矩阵必为偶数阶的.

$$(\mathrm{i}\gamma^\mu\partial_\mu - m)\,\phi(t, \boldsymbol{x}) = 0 \tag{4.14}$$

5 角动量理论

5.1 自旋

Thm. 1 角动量的基本对易关系

$$\left[\hat{J}_i, \hat{J}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{J}_k \tag{5.1}$$

5.2 二态系统

Def. 1 Pauli 矩阵

Pauli 算符 $\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3$ 在 $\hat{\sigma}_3$-表象 ($\hat{S}_z$-表象) 下的矩阵称为 Pauli 矩阵 (Pauli matrices)

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5.2}$$

5.2.1 Pauli 基

Thm. 2 Pauli 基定理

$\{\sigma_0, \sigma_1, \sigma_2, \sigma_3\}$ 构成 $M_2(\mathbb{C})$ 的一个基, 称为 Pauli 基 (Pauli basis). 其中

$$\sigma_0 = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.3}$$

从而任意 2 阶复矩阵 A, 均可由 $\{\sigma_\mu\}_{\mu=0,1,2,3}$ 展开:

$$A = x_0\sigma_0 + \boldsymbol{x}\cdot\boldsymbol{\sigma} = \begin{pmatrix} x_0 + x_3 & x_1 - \mathrm{i}x_2 \\ x_1 + \mathrm{i}x_2 & x_0 - x_3 \end{pmatrix} \tag{5.4}$$

Rmk 若 $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, 则

$$x_0 = \frac{a+d}{2} \quad x_1 = \frac{b+c}{2} \quad x_2 = \mathrm{i}\frac{b-c}{2} \quad x_3 = \frac{a-d}{2} \tag{5.5}$$

Prop. 1 自伴算符与斜自伴算符的 Pauli 算符分解

对任一作用于 2-dim Hilbert 空间上的自伴算符 $\hat{A}$, 其矩阵表示 A 均可以分解为 Pauli 算符 $\{\hat{\sigma}_\mu\}_{\mu=0,1,2,3}$.

$$\hat{A} = x_0\hat{\sigma}_0 + \boldsymbol{x}\cdot\hat{\boldsymbol{\sigma}} \quad (x_\mu \in \mathbb{R}) \tag{5.6}$$

斜自伴算符 $\hat{B}$ 也可以分解为

$$\hat{B} = \mathrm{i}(y_0\hat{\sigma}_0 + \boldsymbol{y}\cdot\hat{\boldsymbol{\sigma}}) \quad (y_\mu \in \mathbb{R}) \tag{5.7}$$

Prop. 2　特殊幺正算符的 Pauli 算符分解

2 阶特殊幺正矩阵 $u \in \mathrm{SO}(2)$ 可以分解为 Pauli 矩阵 $\{\sigma_\mu\}_{\mu=0,1,2,3}$.

$$u = a_0\sigma_0 + \mathrm{i}\boldsymbol{a}\cdot\boldsymbol{\sigma} \quad (a_\mu \in \mathbb{R}) \tag{5.8}$$

Prop. 3　Pauli 矩阵的代数性质

1. 三性合一: σ_i 均自伴、幺正、对合. 从而本征值为 ±1.
2. 对易关系
$$[\sigma_i, \sigma_j] = 2\mathrm{i}\varepsilon_{ijk}\sigma_k \tag{5.9}$$
3. 反对易关系
$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}\sigma_0 \tag{5.10}$$
4. 乘法公式
$$\sigma_i\sigma_j = \delta_{ij}\sigma_0 + \mathrm{i}\varepsilon_{ijk}\sigma_k \tag{5.11}$$
5. 迹
$$\mathrm{tr}\,\sigma_i = 0 \tag{5.12}$$
$$\mathrm{tr}(\sigma_i\sigma_j) = 2\delta_{ij} \tag{5.13}$$
$$\mathrm{tr}(\sigma_i\sigma_j\sigma_k) = 2\mathrm{i}\varepsilon_{ijk} \tag{5.14}$$
6. 行列式
$$\det\sigma_i = -1 \tag{5.15}$$
$$\det(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{v}) = -\boldsymbol{v}^2 \tag{5.16}$$

Rmk　自伴性、幺正性、对合性、对易与反对易关系、乘法结构、本征值、迹、行列式均在幺正相似变换下不变, 因此上述代数结构对于 Pauli 算符 $\hat{\sigma}_i$ 也成立.

Prop. 4　Pauli 矢量恒等式

设 $\left[\hat{\boldsymbol{A}}, \hat{\boldsymbol{\sigma}}\right] = \left[\hat{\boldsymbol{B}}, \hat{\boldsymbol{\sigma}}\right] = 0$, 即 $\hat{\boldsymbol{A}}, \hat{\boldsymbol{B}}$ 均为作用在外部自由度上的矢量算符.

$$\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{A}}\right)\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{B}}\right) = \hat{\boldsymbol{A}}\cdot\hat{\boldsymbol{B}} + \mathrm{i}\hat{\boldsymbol{\sigma}}\cdot\left(\hat{\boldsymbol{A}}\times\hat{\boldsymbol{B}}\right) \tag{5.17}$$

Pf $\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{A}}\right)\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{B}}\right)=\hat{\sigma}_i\hat{A}_i\hat{\sigma}_j\hat{B}_j=\hat{\sigma}_i\hat{\sigma}_j\hat{A}_i\hat{B}_j=(\delta_{ij}\hat{I}_2+\mathrm{i}\varepsilon_{ijk}\hat{\sigma}_k)\hat{A}_i\hat{B}_j=\hat{\boldsymbol{A}}\cdot\hat{\boldsymbol{B}}+\mathrm{i}\hat{\sigma}_k\underbrace{\left(\varepsilon_{kij}\hat{A}_i\hat{B}_j\right)}_{=(\hat{\boldsymbol{A}}\times\hat{\boldsymbol{B}})_k}$

Thm. 3　二态系统的密度算符

$$\hat{\rho}=\frac{1}{2}\left(\hat{I}+\langle\hat{\boldsymbol{\sigma}}\rangle\cdot\hat{\boldsymbol{\sigma}}\right)\tag{5.18}$$

Pf Assume $\rho=a\sigma_0+\boldsymbol{b}\cdot\boldsymbol{\sigma}$. Then $\operatorname{tr}\hat{\rho}=a\operatorname{tr}\sigma_0+b_j\underbrace{\operatorname{tr}\sigma_j}_{=0}=2a=1$, $a=\dfrac{1}{2}$.

$\operatorname{tr}(\hat{\rho}\hat{\sigma}_i)=a\operatorname{tr}\sigma_i+b_j\operatorname{tr}(\sigma_j\sigma_i)=b_j\operatorname{tr}(\delta_{ji}\sigma_0+\mathrm{i}\varepsilon_{jik}\sigma_k)=2\delta_{ji}b_j=2b_i$, $b_i=\dfrac{1}{2}\langle\hat{\sigma}_i\rangle$.

5.2.2　Bloch 球

Def. 2　Bloch 矢量

$$\boldsymbol{n}=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)\tag{5.19}$$

$$\sigma_n=\boldsymbol{n}\cdot\boldsymbol{\sigma}=\begin{pmatrix}n_3 & n_1-\mathrm{i}n_2\\ n_1+\mathrm{i}n_2 & -n_3\end{pmatrix}=\begin{pmatrix}\cos\theta & \sin\theta\mathrm{e}^{-\mathrm{i}\varphi}\\ \sin\theta\mathrm{e}^{\mathrm{i}\varphi} & -\sin\theta\end{pmatrix}\tag{5.20}$$

6 全同粒子与复合系统

identical particles

7 GuoHong's Lecture

Duality, Trinity, Quaternity

1. Hermitian
$$\hat{A}^\dagger = \hat{A}$$
2. Unitary
$$\hat{U}^\dagger = \hat{U}^{-1}$$
3. Involutory
$$\hat{A}^2 = \hat{I}$$
4. Idempotent
$$\hat{A}^2 = \hat{A}$$

Prop. 1 Trinity

A Hermitian unitary operator is necessarily involutory.

Rmk Generally, if an operator satisfies any two of the three properties (Hermiticity, unitarity, involution), it must satisfy the third.

Pf $\hat{A}^\dagger = \hat{A} = \hat{A}^{-1}, \implies \hat{A}^2 = \hat{A}\hat{A} = \hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I}.$

7.1 Eigenvalue Problem

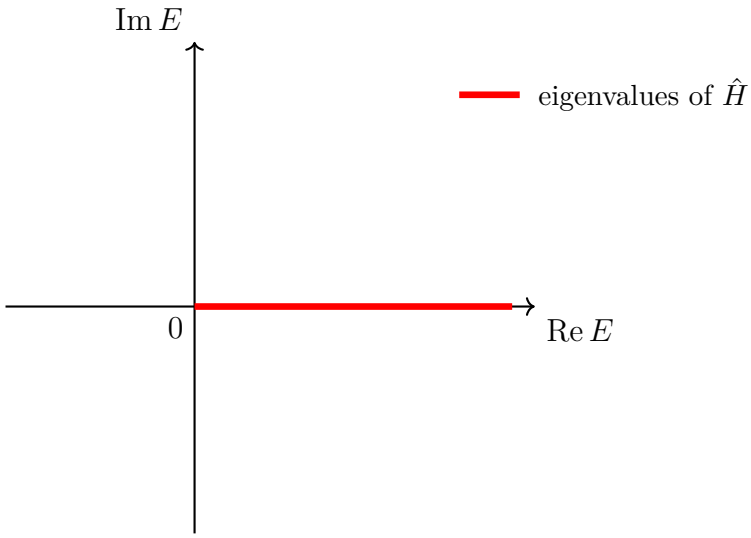
7.1.1 Eigenvalue and Eigenstate

$$\hat{A}\,|\psi\rangle = \lambda\,|\psi\rangle \quad (\lambda \in \mathbb{C})$$

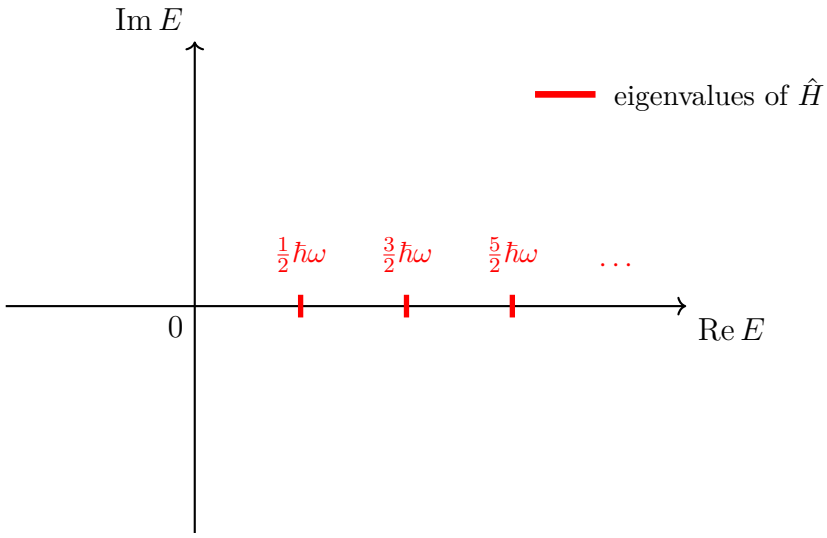
1. Hermitian operator (self-adjoint) $\hat{A}^\dagger = \hat{A}$, observable;
2. Unitary operator $\hat{A}^\dagger = \hat{A}^{-1}$ or $\hat{A}^\dagger\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I}$, symmetric transformation, except for time reversal.

examples of eigenvalues

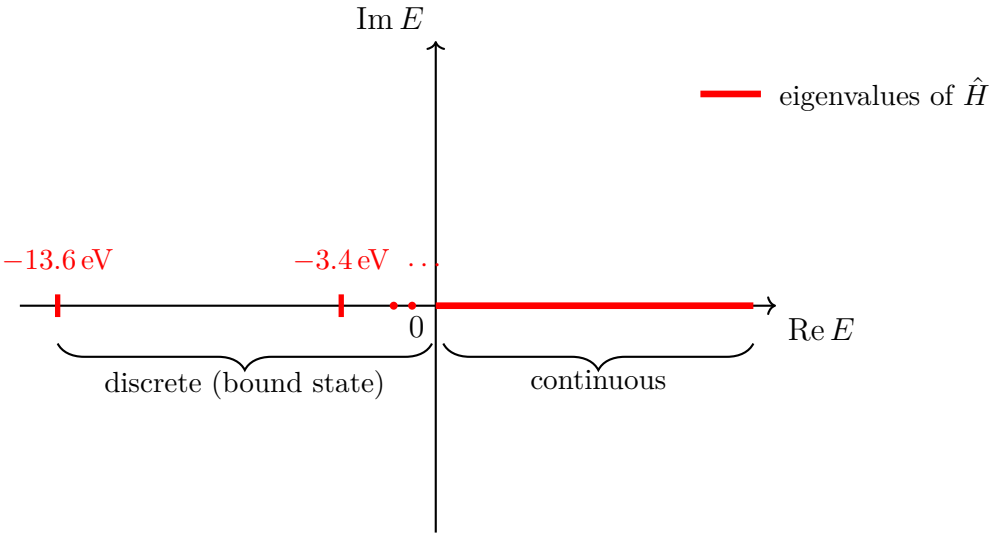
1. free particle: $\hat{H} = \dfrac{\hat{p}^2}{2m}$ (continuous)



2. harmonic oscillator: $\hat{H} = \dfrac{\hat{p}_x}{2m} + \dfrac{1}{2}m\omega^2 x^2$ (discrete)



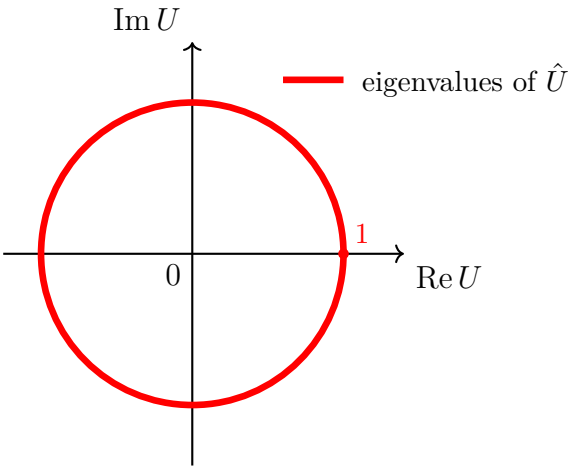
3. hydrogen atom: $\hat{H} = \dfrac{\hat{\boldsymbol{p}}^2}{2m} - \dfrac{e^2}{r}$



4. Unitary operator: Let $\hat{U}\left|u\right\rangle = u\left|u\right\rangle$, $\Rightarrow \left\langle u\right|\hat{U} = \left\langle u\right| u^*$,

$$\Rightarrow \left\langle u\right|\hat{U}^\dagger\hat{U}\left|u\right\rangle = \left\langle u\right| u^* u\left|u\right\rangle = \left|u\right|^2\left\langle u|u\right\rangle = \left\langle u\right|\hat{I}\left|u\right\rangle = \left\langle u|u\right\rangle$$

$\Rightarrow \left|u\right|^2 = 1$, $\Rightarrow u = \mathrm{e}^{\mathrm{i}\theta} \in \mathbb{C}$.



$$\hat{U}^\dagger\left|u\right\rangle = \mathrm{e}^{-\mathrm{i}\theta}\left|u\right\rangle$$

Eigenvalues of Hermitian operators are $\in \mathbb{R}$, and Unitary operators are $\in \mathbb{C}$. The eigenvalues of an operator that is both Hermitian and unitary are $\in \{\pm 1\}$.

Exercises: Proof thms

1. If $\hat{A}^\dagger = \hat{A}$, $\hat{B}^\dagger = \hat{B}$, then $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$ iff $\left[\hat{A}, \hat{B}\right] = 0$.

   Pf $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A} \xrightarrow{\left[\hat{A},\hat{B}\right]=0} \hat{A}\hat{B}$.

2. If $\hat{A}^\dagger = \hat{A}^{-1}$, $\hat{B}^\dagger = \hat{B}^{-1}$, then $(\hat{A}\hat{B})^\dagger = (\hat{A}\hat{B})^{-1}$.

   Pf $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}^{-1}\hat{A}^{-1} = (\hat{A}\hat{B})^{-1}$.

3. If $\hat{A}$ hermitian, then its eigenvalues are real.

   Rmk Let $\hat{A}\left|\psi\right\rangle = a\left|\psi\right\rangle$, then $\left\langle\psi\right|\hat{A}\left|\psi\right\rangle = a\left\langle\psi|\psi\right\rangle = \left\langle\psi\right|\hat{A}\left|\psi\right\rangle^* = a^*\left\langle\psi|\psi\right\rangle$, $\Longrightarrow$ $a = a^*$, $a \in \mathbb{R}$.

4. If $\hat{A}$ is hermitian, then its eigenstates corresponding to distinct eigenvalues are orthogonal. (non-degenerate case)

   Pf Let $\hat{A}\left|\psi\right\rangle = a\left|\psi\right\rangle$, $\hat{A}\left|\psi'\right\rangle = a'\left|\psi'\right\rangle$.

$$\left\langle\psi'\right|\hat{A}\left|\psi\right\rangle = a\left\langle\psi'|\psi\right\rangle = \left\langle\psi'\right|\hat{A}^\dagger\left|\psi\right\rangle = \left(\left\langle\psi\right|\hat{A}\left|\psi'\right\rangle\right) = \left(a'\left\langle\psi|\psi'\right\rangle\right) = a'^*\left\langle\psi'|\psi\right\rangle$$

$\Longrightarrow$ $(a - a')\left\langle\psi'|\psi\right\rangle = 0$, $\xrightarrow{a\neq a'}$ $\left\langle\psi'|\psi\right\rangle = 0$, i.e. $\left|\psi\right\rangle \perp \left|\psi'\right\rangle$. In the degenerate case, one must resort to the Gram-Schmidt orthogonalization procedure.

Thm. 1

Eigenstates of a hermitian operator can form an orthogonal, normalized, complete basis.

- discrete basis (non-degenerate): $\hat{A}\left|\psi_n\right\rangle = a_n\left|\psi_n\right\rangle$.
  - orthonormal: $\langle\psi_n|\psi_m\rangle = \delta_{nm}$
  - complete (meaning the basis is sufficient to span the Hilbert space): $\sum_n \left|\psi_n\right\rangle\left\langle\psi_n\right| = \hat{I}$ (resolution of identity)

  Rmk δ_{nm} is a symmetric tensor.
- continuous basis: $\hat{A}\left|a\right\rangle = a\left|a\right\rangle$
  - orthonormal: $\langle a|a'\rangle = \delta(a-a')$
  - complete: $\int \left|a\right\rangle\left\langle a\right| \mathrm{d}a = \hat{I}$

  Rmk $\delta(a-a')$ is an even function.

7.1.2 Eigenspectrum

Eigenspectrum is the set of eigenvalues.

example of eigenspectrum

1. free particle: $\mathrm{Spec}(\hat{H}) = \{a \mid a \in \mathbb{R}, a > 0\}$
2. harmonic oscillator: $\mathrm{Spec}(\hat{H}) = \left\{\left(n+\frac{1}{2}\right)\hbar\omega \mid n = 0,1,2,\cdots\right\}$.
3. H atom: $\mathrm{Spec}(\hat{H}) = \left\{\frac{1}{n^2}E_{\mathrm{g}} \mid n = 0,1,2,\cdots\right\} \cup \{a \mid a \in \mathbb{R}, a > 0\}$. Mix spectrum.

   Rmk ON: $\langle n,l,m|n',l',m'\rangle = \delta_{nn'}\delta_{ll'}\delta_{mm'}$, $\langle E,l,m|E',l',m'\rangle = \delta(E-E')\delta_{ll'}\delta_{mm'}$.

   RI: $\sum_{n,l,m} \left|n,l,m\right\rangle\left\langle n,l,m\right| + \int \mathrm{d}E \sum_{l,m} \left|E,l,m\right\rangle\left\langle E,l,m\right| = \hat{I}$.
4. Unitary operator: $\mathrm{Spec}(\hat{U}) = \{u \in \mathbb{C} \mid |u| = 1\}$

7.1.3 Eigenspace

Degenerate case (one eigenvalue corresponds to multiple eigenstates):

$$\hat{A}\left|\psi_n^i\right\rangle = a_n\left|\psi_n^i\right\rangle \quad (i = 1,2,\cdots,g_n)$$

where g_n denotes the degeneracy.

Def. 1 Subspace

$$\mathscr{H}_n = \text{Span}\left\{\left|\psi_n^i\right\rangle \mid i = 1, 2, \cdots, g_n\right\}$$

$$\mathscr{H} = \bigoplus_{n=1}^{N} \mathscr{H}_n$$

$$\dim \mathscr{H}_n = g_n,\ \dim \mathscr{H} = \dim \bigoplus_{n=1}^{N} \mathscr{H}_n = \sum_{n=1}^{N} \dim \mathscr{H}_n = \sum_{n=1}^{N} g_n.$$

Direct Sum is for the same observable operator.

$\left[\hat{\boldsymbol{L}}^2, \hat{L}_z\right] = 0$, so $\hat{\boldsymbol{L}}^2$ & $\hat{L}_z$ have the same eigenstate $|l, m_l\rangle$. $\hat{\boldsymbol{L}}^2 |l, m_l\rangle = (l+1)\hbar^2 |l, m_l\rangle$.

$$\begin{cases} l = 0, m_l = 0 & \to |0, 0\rangle \quad (1 \text{ dim}) \\ l = 1, m_l = 0, \pm 1 & \to |1, -1\rangle, |1, 0\rangle, |1, 1\rangle \quad (3 \text{ dim}) \\ \quad \vdots \end{cases}$$

$$\dim \mathscr{H}_{\hat{\boldsymbol{L}}^2} = \sum_{l=0}^{l_{\max}} (2l+1)$$

For bound states, the upper limit $l_{\max}$ is finite and determined by n (eg. $l_{\max} = n - 1$ in H). For unbound states, $l_{\max} \to \infty$.

ON: $\left\langle \psi_n^i \middle| \psi_{n'}^{i'} \right\rangle = \delta_{nn'}\delta_{ii'}$, RI: $\sum_{n=1}^{N} \sum_{i=1}^{g_n} \left|\psi_n^i\right\rangle \left\langle \psi_n^i \right| = \sum_{n=1}^{N} \hat{I}_n = \hat{I}$.

Gram-Schmidt Orthogonalization

$$\begin{cases} \left|\phi_n^1\right\rangle = \left|\chi_n^1\right\rangle = \dfrac{|\psi_n^1\rangle}{\sqrt{\langle \psi_n^1 | \psi_n^2 \rangle}} & \\ \left|\chi_n^2\right\rangle = \left|\psi_n^2\right\rangle - \left\langle \phi_n^1 \middle| \psi_n^2 \right\rangle \left|\phi_n^1\right\rangle & \to \left|\phi_n^2\right\rangle = \dfrac{|\chi_n^2\rangle}{\sqrt{\langle |\chi_n^2\rangle | |\chi_n^2\rangle \rangle}} \\ \quad \vdots & \quad \vdots \\ |\chi_n^{g_n}\rangle = |\psi_n^{g_n}\rangle - \sum_{j=1}^{g_n - 1} \left\langle \phi_n^1 \middle| \psi_n^2 \right\rangle \left|\phi_n^1\right\rangle & \to \left|\phi_n^2\right\rangle = \dfrac{|\chi_n^2\rangle}{\sqrt{\langle |\chi_n^2\rangle | |\chi_n^2\rangle \rangle}} \end{cases}$$

7.2 Tensor Product

Origin: multi-freedom.

1. Multi particles: s_1, s_2;
2. Single particle, but multi observables $(\hat{\boldsymbol{L}}^2, \hat{L}_z, \hat{\boldsymbol{S}}^2, \hat{S}_z)$
3. Single particle, single observable, but multi components $(\hat{\boldsymbol{x}} \to \hat{x}, \hat{y}, \hat{z})$

Def. 2 Tensor Product

$|\psi\rangle_1 \in \mathscr{H}_1$, $|\phi\rangle_2 \in \mathscr{H}_2$, then $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$, and $|\chi\rangle = |\psi\rangle_1 \otimes |\phi\rangle_2 \in \mathscr{H}$.

7.2.1 Properties of tensor product

The subscript "i" indicates that the vector $|\psi\rangle_i$ belongs to the subspace $\mathscr{H}_i$.

1. Commutativity

$$|\psi\rangle_1 \otimes |\phi\rangle_2 = |\phi\rangle_2 \otimes |\psi\rangle_1$$

2. Linear: $\forall c \in \mathbb{C}$, $|\psi\rangle_1 \in \mathscr{H}_1, |\phi\rangle_2 \in \mathscr{H}_2$,

$$c(|\psi\rangle_1 \otimes |\phi\rangle_2) = (c\,|\psi\rangle_1) \otimes |\phi\rangle_2 = |\psi\rangle_1 \otimes (c\,|\phi\rangle_2)$$

3. Distributivity

$$(a\,|\psi_1\rangle_1 + b\,|\psi_2\rangle_1) \otimes |\phi\rangle_2 = a\,|\psi_1\rangle_1 \otimes |\phi\rangle_2 + b\,|\psi_2\rangle_1 \otimes |\phi\rangle_2$$

$$|\psi\rangle_1 \otimes (a\,|\phi_1\rangle_2 + b\,|\phi_2\rangle_2) = a\,|\psi\rangle_1 \otimes |\phi_1\rangle_2 + b\,|\psi\rangle_1 \otimes |\phi_2\rangle_2$$

Let $\mathscr{H}_1 = \text{Span}\{|u_i\rangle_1 \mid i = 1, 2, \cdots, N_1\}$, $\mathscr{H}_2 = \text{Span}\{|v_j\rangle_2 \mid j = 1, 2, \cdots, N_2\}$, then $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$,

$$\dim \mathscr{H} = \dim \mathscr{H}_1 \cdot \dim \mathscr{H}_2 = N_1 N_2$$

Let $|\psi\rangle_1 = \sum_i c_i\,|u_i\rangle_1$, $|\phi\rangle_2 = \sum_j d_j\,|v_j\rangle_2$,

$$|\psi\rangle_1 \otimes |\phi\rangle_2 = \left(\sum_i c_i\,|u_i\rangle_1\right) \otimes \left(\sum_j d_j\,|v_j\rangle_2\right) = \sum_{i,j} c_i d_j\,|u_i\rangle_1 \otimes |v_j\rangle_2$$

Let $\mathscr{H}_1 = \text{Span}\{|u_1\rangle_1, |u_2\rangle_1\}$, $\mathscr{H}_2 = \text{Span}\{|v_1\rangle_2, |v_2\rangle_2\}$, then

$$|\psi\rangle_1 \otimes |\phi\rangle_2 = c_1 d_1\,|u_1\rangle_1 \otimes |v_1\rangle_2 + c_1 d_2\,|u_1\rangle_1 \otimes |v_2\rangle_2 + c_2 d_1\,|u_2\rangle_1 \otimes |v_1\rangle_2 + c_2 d_2\,|u_2\rangle_1 \otimes |v_2\rangle_2$$

For a state vector $|\chi\rangle$ $\dfrac{1}{\sqrt{2}}(|u_1\rangle_1 \otimes |v_1\rangle_2 + |u_2\rangle_1 \otimes |v_2\rangle_2) \in \mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$. Ask: do we have proper values of c_1, d_1, c_2, d_2 to match the requirement of $|\chi\rangle$? Answer: NO! $|\chi\rangle \neq |\psi\rangle_1 \otimes |\phi\rangle_2$.

$|\psi\rangle_1 \otimes |\phi\rangle_2$ is called tensor product state. $|\chi\rangle$ is called entangled state.

7.2.2 Entangled State

Eg. 1 Kinds of Entangled State

$N = 2$, $\frac{1}{\sqrt{2}}\left(|u_1\rangle_1 \otimes |v_1\rangle_2 \pm |u_2\rangle_1 \otimes |v_2\rangle_2\right)$ is called Bell-state (Bell basis), or EPR state, or Schrödinger's cat state.
$N \geq 3$:

1. Werner state (W-state): robust
2. GHZ state: fragile
3. NOON state

Two spin system $\left(\frac{1}{2} \otimes \frac{1}{2}\right)$. singlet: 1-entangled state. triplet: 2-tensor product state + 1-entangled state.

7.2.3 Inner product of tensor product

$$\left({}_1\langle\psi_2| \otimes {}_2\langle\phi_2|\right)\left(|\psi_1\rangle_1 \otimes |\phi_1\rangle_2\right) = \left({}_1\langle\psi_2|\psi_1\rangle_1\right)\left({}_2\langle\phi_2|\phi_1\rangle_2\right)$$

$$\left({}_1\langle u_i| \otimes {}_2\langle v_j|\right)\left(|u_k\rangle_1 \otimes |v_l\rangle_2\right) = \left({}_1\langle u_i|u_k\rangle_1\right)\left({}_2\langle v_j|v_l\rangle_2\right) = \delta_{ik}\delta_{jl}$$

If $\hat{A}$ acts only on $\mathscr{H}_1$, i.e. $\hat{A} \to |\psi\rangle_1$, and $\hat{B}$ acts only on $\mathscr{H}_2$, i.e. $\hat{B} \to |\phi\rangle_2$. Then $\hat{A} = \hat{A}_1 \otimes \hat{I}_2$, $\hat{B} = \hat{I}_1 \otimes \hat{B}_2$.

$$\hat{A}(|\psi\rangle_1 \otimes |\phi\rangle_2) = (\hat{A}_1 \otimes \hat{I}_2)(|\psi\rangle_1 \otimes |\phi\rangle_2) = \hat{A}_1 |\psi\rangle_1 \otimes \hat{I}_2 |\phi\rangle_2 = (\hat{A}_1 |\psi\rangle_1) \otimes |\phi\rangle_2$$

$$\hat{B}(|\psi\rangle_1 \otimes |\phi\rangle_2) = (\hat{I}_1 \otimes \hat{B}_2)(|\psi\rangle_1 \otimes |\phi\rangle_2) = \hat{I}_1 |\psi\rangle_1 \otimes \hat{B}_2 |\phi\rangle_2 = |\psi\rangle_1 \otimes (\hat{B}_2 |\phi\rangle_2)$$

The operator has no effect on the space on which it does not act.

Eg. 2 Momentum

For $\hat{\boldsymbol{p}}^2 |\boldsymbol{p}\rangle = \boldsymbol{p}^2 |\boldsymbol{p}\rangle$, $|\boldsymbol{p}\rangle = |p_x\rangle \otimes |p_y\rangle \otimes |p_z\rangle$, $\hat{p}_x^2 = \hat{p}_x^2 \otimes \hat{I}_y \otimes \hat{I}_z$, the same as y, z.

Eg. 3 Angular Momentum

Let $\hat{\boldsymbol{L}}^2 \to l$, $\hat{L}_z \to m_l$, $\hat{\boldsymbol{S}}^2 \to s$, $\hat{S}_z \to m_s$. $\mathscr{H}_l = |l, m_l\rangle$, $\mathscr{H}_s = |s, m_s\rangle$, $\mathscr{H} = \mathscr{H}_l \otimes \mathscr{H}_s$. Fix $l, s = 1/2$, then

$$\dim \mathscr{H} = \dim \mathscr{H}_l \cdot \dim \mathscr{H}_s = (2l+1)(2s+1) = 2(2l+1)$$

Eg. 4 Hydrogen Atom*

nL_j. n is principle, L_j is spectrum

7.3 Compatible Observable

1. Compatible observable (CO) is commuting observable, i.e. $\left[\hat{A},\hat{B}\right]=0$.
2. Common eigenstate (CE) or simultaneous eigenstate (SE)
3. Set of common eigenstate (SCE)
4. Complete set of commuting observable (CSCO)
5. Good quantum numbers (GQN)
6. Diagonal matrix. Block diagonal matrix. Diagonalization of matrix.

Thm of Compatible Observable:

$$\left[\hat{A},\hat{B}\right]=0 \quad\Longleftrightarrow\quad \begin{cases}\hat{A},\hat{B}\text{ have SCE}\\ \text{orthogonal basis}\end{cases}$$

$$\left[\hat{A}_i,\hat{A}_j\right]=0,\qquad (i,j=1,2,\ldots,n)\Longleftrightarrow\begin{cases}①\text{ SCE (SSE)},\\ ②\text{ ON.}\end{cases}$$

$$\left[\hat{A}_i,\hat{A}_j\right]=0,\qquad \left[\hat{A}_i,\hat{B}\right]=0,\qquad (i,j=1,2,\ldots,n)\Longrightarrow\text{CSCO.}$$

diagonal matrix:

$$\hat{A}=\operatorname{diag}\left(\underbrace{\lambda_1,\ldots,\lambda_1}_{g_1},\ldots,\underbrace{\lambda_n,\ldots,\lambda_n}_{g_n}\right),\qquad g_i\ (i=1,2,\ldots,n)\text{ degeneracy.}$$

block diagonal matrix:

$$\hat{B}=\operatorname{diag}\left(B_1,B_2,\ldots,B_n\right),\qquad B_i:\ g_i\times g_i.$$

$$\begin{cases}\hat{L}^2=\hbar^2\operatorname{diag}\left(0,2,2,2,6,6,6,6,6,\ldots\right).\\ \hat{L}_z=\hbar\operatorname{diag}\left(0,-1,0,1,-2,-1,0,+1,+2,\ldots\right).\end{cases}$$

[Proof]

Suppose

$$\left[\hat{A},\hat{B}\right]=0,\qquad \hat{A}\left|\psi\right\rangle=\lambda\left|\psi\right\rangle.$$

Then

$$\hat{A}\big(\hat{B}\,|\psi\rangle\big) = \hat{B}\hat{A}\,|\psi\rangle = \lambda\big(\hat{B}\,|\psi\rangle\big).$$

Thus, $\hat{B}\,|\psi\rangle$ is eigenstate of $\hat{A}$ with the eigenvalue of λ.

① Suppose λ is non-degenerate. Then

$$\hat{B}\,|\psi\rangle = \mu\,|\psi\rangle \sim |\psi\rangle\,.$$

② If λ_n is degenerate, then

$$\hat{A}\left|\psi_n^i\right\rangle = \lambda_n\left|\psi_n^i\right\rangle, \qquad i = 1, 2, \cdots, g_n.$$

$$\langle\psi_n^i|\psi_m^j\rangle = \delta_{nm}\delta_{ij} \qquad (n = 1, 2, \cdots, g_n;\ j = 1, 2, \cdots, g_m)$$

$$\begin{cases} \langle\psi_n^i|\hat{A}\hat{B}|\psi_m^j\rangle = \lambda_m\langle\psi_n^i|\hat{B}|\psi_m^j\rangle, \\ \langle\psi_n^i|\hat{B}\hat{A}|\psi_m^j\rangle = \lambda_n\langle\psi_n^i|\hat{B}|\psi_m^j\rangle \end{cases} \qquad [\hat{A}, \hat{B}] = 0$$

$$(\lambda_n - \lambda_m)\langle\psi_n^i|\hat{B}|\psi_m^j\rangle = 0$$

$$n \neq m \Longrightarrow \lambda_n \neq \lambda_m \Longrightarrow \langle\psi_n^i|\hat{B}|\psi_m^j\rangle = 0 \Longrightarrow \hat{B} \text{ is a block diagonal}$$

$$B_{ij}^{(n)} = \langle\psi_n^i|\hat{B}|\psi_n^j\rangle$$

$$\hat{B}^{(n)}|\varphi_n^i\rangle = \mu_i^{(n)}|\varphi_n^i\rangle. \Longrightarrow \langle\varphi_n^i|\hat{B}^{(n)}|\varphi_n^j\rangle = \mu_i^{(n)}\delta_{ij}$$

$\hat{B}^{(n)}$: $g_n \times g_n$ diagonal matrix.

$$|\varphi_n^i\rangle = \mathbb{I}|\varphi_n^i\rangle = \left(\sum_j |\psi_n^j\rangle\langle\psi_n^j|\right)|\varphi_n^i\rangle = \sum_j \Big(\langle\psi_n^j|\varphi_n^i\rangle\Big)\,|\psi_n^j\rangle$$

$$\Rightarrow \hat{A}|\varphi_n^i\rangle = \hat{A}\left[\sum_j \Big(\langle\psi_n^j|\varphi_n^i\rangle\Big)\,|\psi_n^j\rangle\right] = \lambda_n\left[\sum_j \Big(\langle\psi_n^j|\varphi_n^i\rangle\Big)\,|\psi_n^j\rangle\right] = \lambda_n|\varphi_n^i\rangle.$$

SCE of $\hat{A}$ and $\hat{B}$ $\left|\phi_{n,k}^i\right\rangle$

$$\begin{cases} \hat{A}|\varphi_{n,k}^i\rangle = \lambda_n|\varphi_{n,k}^i\rangle \\ \hat{B}|\varphi_{n,k}^i\rangle = \mu_k|\varphi_{n,k}^i\rangle \end{cases} \Rightarrow \begin{cases} \hat{A}\hat{B}|\varphi_{n,k}^i\rangle = \mu_k\lambda_n|\varphi_{n,k}^i\rangle \\ \hat{B}\hat{A}|\varphi_{n,k}^i\rangle = \lambda_n\mu_k|\varphi_{n,k}^i\rangle \end{cases} \Rightarrow [\hat{A}, \hat{B}]|\varphi_{n,k}^i\rangle = 0.$$

$\forall|\psi\rangle$,

$$|\psi\rangle=\sum_n C_n|\varphi^i_{n,k}\rangle \Rightarrow [\hat{A},\hat{B}]|\psi\rangle=\sum_n C_n[\hat{A},\hat{B}]|\varphi^i_{n,k}\rangle=0\Rightarrow[\hat{A},\hat{B}]=0.$$

7.4 Representation Transformation

7.4.1 Wavefunction

The wave-function is the projection of the state-vector in a certain rep.

$\hat{\boldsymbol{x}}$-rep: $\hat{\boldsymbol{x}}\,|\boldsymbol{x}\rangle=\boldsymbol{x}\,|\boldsymbol{x}\rangle$. $\begin{cases}\langle\boldsymbol{x}|\boldsymbol{x}'\rangle=\delta(\boldsymbol{x}-\boldsymbol{x}') & \text{ON}\\ \int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|=\hat{I} & \text{RI}\end{cases}$

$$|\psi\rangle=\hat{I}\,|\psi\rangle=\left(\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\right)|\psi\rangle=\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\,\psi(\boldsymbol{x})$$

where $\psi(\boldsymbol{x})=\langle\boldsymbol{x}|\psi\rangle$ is wavefunction in $\boldsymbol{x}$-rep.

$\boldsymbol{p}$-rep: $\hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle=\boldsymbol{p}\,|\boldsymbol{p}\rangle$. $\begin{cases}\langle\boldsymbol{p}|\boldsymbol{p}'\rangle=\delta(\boldsymbol{p}-\boldsymbol{p}') & \text{ON}\\ \int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}|=\hat{I} & \text{RI}\end{cases}$

$$|\psi\rangle=\left(\int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}|\right)|\psi\rangle=\int \mathrm{d}^3p\,|\boldsymbol{p}\rangle\,\tilde{\psi}(\boldsymbol{p})$$

where $\tilde{\psi}(\boldsymbol{p})=\langle\boldsymbol{p}|\psi\rangle$.

$$|\psi\rangle=\left(\sum_j |u_n\rangle\langle u_n|\right)|\psi\rangle=\sum_n c_n\,|u_n\rangle$$

where $c_n=\langle u_n|\psi\rangle$ is the wavefunction in $\{|u_n\rangle\}$-rep or $\hat{A}$-rep, if $\hat{A}\,|u_n\rangle=A_n\,|u_n\rangle$.

7.4.2 Representation Transformation

$$|\psi\rangle=\int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\,\tilde{\psi}(\boldsymbol{p})=\int \mathrm{d}^3x\ \underbrace{\left(\int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}|\right)}_{=\hat{I}}\psi(\boldsymbol{x})=\int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\int \mathrm{d}^3x\,\psi(\boldsymbol{x})\,\langle\boldsymbol{p}|\boldsymbol{x}\rangle$$

$$\Longrightarrow \tilde{\psi}(\boldsymbol{p})=\int \mathrm{d}^3x\,\psi(\boldsymbol{x})=\psi^*_{\boldsymbol{p}}(\boldsymbol{x})$$

where $\psi_{\boldsymbol{p}}(\boldsymbol{x})=\langle\boldsymbol{x}|\boldsymbol{p}\rangle$.

$$\psi(\boldsymbol{x})=\tilde{\psi}(\boldsymbol{p})\psi_{\boldsymbol{p}}(\boldsymbol{x})$$

The key is $\langle\boldsymbol{x}|\boldsymbol{p}\rangle$ and $\langle\boldsymbol{p}|\boldsymbol{x}\rangle$

In $\hat{\boldsymbol{x}}$-rep,

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = \psi_{\boldsymbol{p}}(\boldsymbol{x}) = N\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \qquad (\Longleftrightarrow \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla)$$

where N is the normalization factor.

In $\hat{\boldsymbol{p}}$-rep, $\hat{\boldsymbol{x}} = +\mathrm{i}\hbar\nabla_{\boldsymbol{p}} \Longleftrightarrow \langle \boldsymbol{p}|\boldsymbol{x}\rangle = N\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}$.

How to determine the normalization factor?

$$\langle \boldsymbol{x}|\boldsymbol{x}'\rangle = \delta(\boldsymbol{x}-\boldsymbol{x}') = \int \mathrm{d}^3p\ \langle \boldsymbol{x}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\boldsymbol{x}'\rangle = N^2\int \mathrm{d}^3p\,\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}$$

$$\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k = 2\pi\delta(x) \quad \Longrightarrow \langle \boldsymbol{x}|\boldsymbol{x}'\rangle = M^2(2\pi\hbar)^3\delta(\boldsymbol{x}-\boldsymbol{x}') \quad \Longrightarrow N = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}$$

$$\Longrightarrow \langle \boldsymbol{x}|\boldsymbol{p}\rangle = \psi_{\boldsymbol{p}}(\boldsymbol{x}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \qquad (\Longleftrightarrow \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla)$$

$\hat{x}$-representation	$\hat{p}$-representation
$\hat{x} = \hat{x}, \quad \hat{p} = -\mathrm{i}\hbar\nabla_x$	$\hat{p} = \hat{p}, \quad \hat{x} = +\mathrm{i}\hbar\nabla_p$
$\hat{x}\,\lvert\boldsymbol{x}\rangle = \boldsymbol{x}\,\lvert\boldsymbol{x}\rangle$	$\hat{p}\,\lvert\boldsymbol{p}\rangle = \boldsymbol{p}\,\lvert\boldsymbol{p}\rangle$
$\hat{x}\delta(\boldsymbol{x}-\boldsymbol{x}') = \boldsymbol{x}'\delta(\boldsymbol{x}-\boldsymbol{x}')$	$\hat{p}\delta(\boldsymbol{p}-\boldsymbol{p}') = \boldsymbol{p}'\delta(\boldsymbol{p}-\boldsymbol{p}')$
$\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle \boldsymbol{x}|\boldsymbol{p}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}$	$\psi_{\boldsymbol{x}}(\boldsymbol{p}) = \langle \boldsymbol{p}|\boldsymbol{x}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}}\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}$

7.4.3 Schrödinger eq

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\lvert\psi(t)\rangle = \hat{H}\lvert\psi(t)\rangle = \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}})\right]\lvert\psi(t)\rangle$$

In $\hat{\boldsymbol{x}}$-rep,

$$\Longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)$$

where $\psi(\boldsymbol{x},t) = \langle \boldsymbol{x}|\psi(t)\rangle$.

In $\hat{\boldsymbol{p}}$-rep,

$$\Longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}\tilde{\psi}(\boldsymbol{p},t) = \frac{\hat{\boldsymbol{p}}^2}{2m}\tilde{\psi}(\boldsymbol{p},t) + V(\mathrm{i}\hbar\nabla_{\boldsymbol{p}})\tilde{\psi}(\boldsymbol{p},t)$$

where $\tilde{\psi}(\boldsymbol{p},t) = \langle \boldsymbol{p}|\psi(t)\rangle$.

7.5 Adjoint

$\hat{A}^\dagger = (\hat{A}^{\mathrm{T}})^*$ 不一定对每个算符成立, 有些算符不能写成矩阵. 原始定义为

$$(\hat{A}\lvert\psi\rangle)^\dagger = \langle\psi\rvert\hat{A}^\dagger \quad \Longleftrightarrow \quad \langle\psi\rvert\hat{A}^\dagger\lvert\phi\rangle = \langle\phi\rvert\hat{A}\lvert\psi\rangle^*$$

Pf $|\psi\rangle = \sum_n c_n |u_n\rangle\,, \qquad |\phi\rangle = \sum_m d_m |u_m\rangle\,.$

$$\langle\psi|\hat{A}^\dagger|\phi\rangle = \sum_{n,m}\langle u_n| c_n^* \hat{A}^\dagger d_m |u_m\rangle = \sum_{n,m} c_n^* d_m \langle u_n|\hat{A}^\dagger|u_m\rangle = \sum_{n,m} c_n^* d_m \left(\hat{A}^\dagger\right)_{nm}.$$

$$\left(\langle\phi|\hat{A}|\psi\rangle\right)^* = \left[\sum_{n,m}\langle u_m| d_m^* \hat{A} c_n |u_n\rangle\right]^* = \left[\sum_{n,m} d_m^* c_n \left(\hat{A}\right)_{mn}\right]^* = \sum_{n,m} d_m c_n^* \left(\hat{A}\right)^*_{mn}.$$

$$\Longrightarrow \quad \left(\hat{A}^\dagger\right)_{nm} = \left(\hat{A}\right)^*_{mn} = \left(\hat{A}^\intercal\right)^*_{nm}. \quad \Longrightarrow \quad \hat{A}^\dagger = \left(\hat{A}^\intercal\right)^*.$$

Adjoint = transpose + complex conjugate.

7.6 Unitary and Anti-unitary

$$\text{space (spacial)} \begin{cases} \text{translation} & \text{momentum conservation} \\ \text{reflection (parity inversion)} & \text{party conservation} \\ \text{rotation} & \text{angular momentum conservation} \end{cases}$$

$$\text{time (temporary)} \begin{cases} \text{translation} & \text{energy} \\ \text{reversal} & \text{no conservation but Kramer's degeneracy} \end{cases}$$

Time reversal is anti-linear and anti-unitary.