

量子力学混合态表象*

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(2014年4月18日收到; 2014年5月26日收到修改稿)

在以往的文献中量子力学的表象都是纯态表象, 在本文中我们从算符的合理排序和概率统计的正态分布思想出发, 首次提出了量子力学混合态表象的概念, 并证明了其完备性和正交性. 量子力学混合态表象的优点是可以反映算符的多种表示以及其相应的排序规则.

关键词: 量子力学混合态表象, 量子力学纯态表象, 排序规则, IWOP技术

PACS: 03.65.-w, 42.50.-p

DOI: 10.7498/aps.63.190302

1 引言

自从狄拉克建立量子力学的表象理论以后, 人们对量子论的理解得以深化. 以往文献中都是纯态表象, 其存在条件是完备性^[1]. 例如我们以 Q 表示坐标算符, 以 $|q\rangle$ 表示其本征态, 狄拉克的坐标表象的完备性记为

$$\int_{-\infty}^{\infty} dq |q\rangle \langle q| = 1, \quad (1)$$

这里 $|q\rangle \langle q|$ 是纯态; 动量表象的完备性是

$$\int_{-\infty}^{\infty} dp |p\rangle \langle p| = 1, \quad (2)$$

$|p\rangle \langle p|$ 是纯态, $|p\rangle$ 是动量算符 P 的本征态, $[Q, P] = i\hbar$; 量子光学中常用的相干态表象的超完备性是^[2]

$$\int \frac{d^2z}{\pi} |z\rangle \langle z| = 1, \quad (3)$$

$|z\rangle \langle z|$ 也是纯态. 那么混合态(密度矩阵)能不能构成表象呢? 如果能, 混合态表象有什么特点呢? 这些问题在以往的文献中未见有报道. 在本文中我们从概率统计的正态分布思想出发, 首次提出量子混合态表象的概念, 然后我们应用算符的合理排序技术提出混合态表象, 并给出其特点和应用.

2 混合态表象的提出

参考数理统计中随机变量的正态分布的思想, 我们在 (q, p) 相空间中引入正规乘积形式的正态分布算符 $\Delta_g(q, p)$

$$\begin{aligned} \Delta_g(q, p) = & \frac{1}{2\pi\sqrt{1-\tau^2}} : \exp \left\{ -\frac{1}{2(1-\tau^2)} \right. \\ & \times \left[\frac{(q-Q)^2}{\sigma_1^2} - 2\tau \frac{(q-Q)(p-P)}{\sigma_1\sigma_2} \right. \\ & \left. \left. + \frac{(p-P)^2}{\sigma_2^2} \right] \right\} :, \end{aligned} \quad (4)$$

这是一个混合态, 它不能表达为 $|\rangle \langle|$ 的形式. 令

$$\begin{aligned} \Lambda = 1 - \tau^2, \quad \sigma_p = \frac{1}{\sigma_1^2}, \\ \sigma_q = \frac{1}{\sigma_2^2}, \quad \sigma_{q,p} = \frac{\tau}{\sigma_1\sigma_2}, \end{aligned} \quad (5)$$

则

$$\begin{aligned} \Delta_g(q, p) = & (2\pi\sqrt{\Lambda})^{-1} : \exp \{ -[\sigma_p(q-Q)^2 - 2\sigma_{q,p} \\ & \times (q-Q)(p-P) + \sigma_q(p-P)^2] / 2\Lambda \} :. \end{aligned} \quad (6)$$

注意到

$$\sigma_q\sigma_p - \sigma_{q,p}^2 = \frac{1-\tau^2}{(\sigma_1\sigma_2)^2} = \frac{\Lambda}{(\sigma_1\sigma_2)^2} > 0, \quad (7)$$

* 国家自然科学基金(批准号: 11175113, 11275123)资助的课题.

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这是正态分布的必要条件.

3 混合态 $\Delta_g(q, p)$ 的性质

用有序算符内的积分技术^[3-7]可以证明

$$\frac{1}{\sigma_1\sigma_2} \iint_{-\infty}^{\infty} dpdq \Delta_g(q, p) = 1, \quad (8)$$

这是混合态表象的完备性. 事实上

$$\begin{aligned} & \frac{1}{\sigma_1\sigma_2} \iint_{-\infty}^{\infty} \Delta_g(q, p) dq dp \\ &= (2\pi\sigma_1\sigma_2\sqrt{\Lambda})^{-1} \iint_{-\infty}^{\infty} : \exp\{-[\sigma_p(q-Q)^2 - 2\sigma_{q,p} \\ & \quad \times (q-Q)(p-P) + \sigma_q(p-P)^2]/2\Lambda\} : dq dp \\ &= (2\pi\sigma_1\sigma_2\sqrt{\Lambda})^{-1} \sqrt{\frac{2\pi\Lambda}{\sigma_p}} \\ & \quad \times \int : e^{\frac{\sigma_{q,p}^2(p-P)^2}{2\Lambda\sigma_p} - \frac{\sigma_q}{2\Lambda}(p-P)^2} : dp \\ &= (\sqrt{2\pi\sigma_p})^{-1} \sqrt{\frac{2\pi\Lambda\sigma_p}{\sigma_q\sigma_p - \sigma_{q,p}^2}} \\ &= (\sigma_1\sigma_2)^{-1} \sqrt{\frac{\Lambda}{\sigma_q\sigma_p - \sigma_{q,p}^2}} \\ &= (\sigma_1\sigma_2)^{-1} \sqrt{\frac{\Lambda(\sigma_1\sigma_2)^2}{\Lambda}} \\ &= 1. \end{aligned} \quad (9)$$

因此任何算符 H 可以用它做展开,

$$H = \frac{1}{\sigma_1\sigma_2} \iint_{-\infty}^{\infty} \Delta_g(q, p) h(q, p) dq dp, \quad (10)$$

形成 H 在此混合态表象中的表示函数 $h(q, p)$, 我们将在稍后求出它. 由

$$\begin{aligned} & \iint_{-\infty}^{\infty} : (q-Q)(p-P) \Delta_g(q, p) : dq dp \\ &= \tau\sigma_q\sigma_p, \end{aligned} \quad (11)$$

可知 τ 代表用 Q 测量和用 P 测量之间的关联. 当 $\tau = 0$, $\Delta_g(q, p)$ 约化为两个独立的单变量正态分布的乘积

$$\begin{aligned} & \Delta_g(q, p)|_{\tau=0} \rightarrow \frac{1}{2\pi\sigma_1\sigma_2} \\ & \quad \times : \exp\left\{-\frac{(q-Q)^2}{2\sigma_1^2} - \frac{(p-P)^2}{2\sigma_2^2}\right\} :. \end{aligned} \quad (12)$$

然后我们计算混合态表象的边缘分布

$$\begin{aligned} & \int_{-\infty}^{\infty} \Delta_g(q, p) dp \\ &= (2\pi\sqrt{\Lambda})^{-1} \sqrt{\frac{2\pi\Lambda}{\sigma_p}} : e^{\frac{\sigma_{q,p}^2 - \sigma_q\sigma_p}{2\Lambda\sigma_p}(p-P)^2} : \\ &= (\sqrt{2\pi\sigma_p})^{-1} : e^{-\frac{1}{2\sigma_p}(p-P)^2} : \end{aligned} \quad (13)$$

和

$$\begin{aligned} & \int_{-\infty}^{\infty} \Delta_g(q, p) dq \\ &= (\sqrt{2\pi\sigma_q})^{-1} : e^{-\frac{1}{2\sigma_q}(q-Q)^2} :. \end{aligned} \quad (14)$$

4 混合态表象所体现的三种算符排序

令

$$\begin{aligned} & \sigma_1 = \sigma_2 = \frac{1}{\sqrt{2}}, \quad \tau = -ik, \\ & 2(1 - \tau^2)\sigma_1^2 = 1 + k^2, \\ & \frac{\tau}{(1 - \tau^2)\sigma_1\sigma_2} = -\frac{2ik}{1 + k^2}, \end{aligned} \quad (15)$$

就可将 $\Delta_g(q, p)$ 改写为

$$\begin{aligned} & \Omega_k(p, q) \\ &= \frac{1}{2\pi\sqrt{(1+k^2)}} : \exp\left\{-\frac{(q-Q)^2}{1+k^2} - \frac{2ik}{1+k^2} \right. \\ & \quad \left. \times (q-Q)(p-P) - \frac{(p-P)^2}{1+k^2}\right\} :. \end{aligned} \quad (16)$$

结合数理统计的理论分析 (A1) 式 (见附录), 看出参数 k 起的作用是关联 Q 和 P , 这也可以从以下积分证实:

$$\iint dpdq : (q-Q)(p-P) \Omega_k(p, q) : = -4ik. \quad (17)$$

当 $k = 0$

$$\Omega_{k=0}(p, q) = \frac{1}{\pi} : e^{-(q-Q)^2 - (p-P)^2} :, \quad (18)$$

这正好是 Wigner 算符的正规乘积形式^[8], 对应算符的 Weyl 排序. 当 $k = 1$, 鉴于

$$|p\rangle = \pi^{-1/4} \exp\left[-\frac{p^2}{2} + \sqrt{2}ipa^\dagger + \frac{a^{\dagger 2}}{2}\right] |0\rangle, \quad (19)$$

$$|q\rangle = \pi^{-1/4} \exp\left[-\frac{q^2}{2} + \sqrt{2}qa^\dagger - \frac{a^{\dagger 2}}{2}\right] |0\rangle, \quad (20)$$

$|0\rangle$ 是 Fock 空间的真空态, 以及

$$|0\rangle\langle 0| =: e^{-aa^\dagger} :, \quad (21)$$

可知

$$\Omega_{k=1}(p, q)$$

$$\begin{aligned}
 &= \frac{1}{\pi\sqrt{2}} : \exp \left\{ -\frac{(q-Q)^2}{2} - \frac{i}{2} \right. \\
 &\quad \left. \times (q-Q)(p-P) - \frac{(p-P)^2}{2} \right\} : \\
 &= \frac{1}{\sqrt{2\pi}} |p\rangle\langle q| e^{-ipq}. \tag{22}
 \end{aligned}$$

它又等于

$$\frac{1}{\sqrt{2\pi}} |q\rangle\langle p| e^{ipq} = \delta(q-Q)\delta(p-P). \tag{23}$$

体现了 $Q-P$ 排序的积分核^[9], 例如

$$\begin{aligned}
 &Q^n P^m \\
 &= Q^n \int_{-\infty}^{\infty} dq |q\rangle\langle q| \int_{-\infty}^{\infty} dp |p\rangle\langle p| P^m \\
 &= \frac{1}{\sqrt{2\pi}} \iint_{-\infty}^{\infty} dp dq q^n p^m |q\rangle\langle p| e^{ipq} \\
 &= \iint_{-\infty}^{\infty} dp dq q^n p^m \delta(q-Q)\delta(p-P). \tag{24}
 \end{aligned}$$

而当 $k = -1$,

$$\Omega_{k=-1}(p, q) = \frac{1}{\sqrt{2\pi}} |q\rangle\langle p| e^{ipq}, \tag{25}$$

$$\frac{1}{\sqrt{2\pi}} |q\rangle\langle p| e^{ipq} = \delta(q-Q)\delta(p-P). \tag{26}$$

体现了 $P-Q$ 排序^[9]. 即

$$\begin{aligned}
 P^m Q^n &= P^m \int_{-\infty}^{\infty} dp |p\rangle\langle p| \int_{-\infty}^{\infty} dq |q\rangle\langle q| Q^n \\
 &= \frac{1}{\sqrt{2\pi}} \iint_{-\infty}^{\infty} dp dq |p\rangle\langle q| e^{-ipq} p^m q^n. \tag{27}
 \end{aligned}$$

5 混合态 $\Omega_k(p, q)$ 在坐标表象的形式

注意到动量本征态的 Fourier 变换

$$\begin{aligned}
 \langle p| &= \int_{-\infty}^{\infty} dq' \langle p|q'\rangle \langle q'| \\
 &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq' e^{-ipq'} \langle q'| \tag{28}
 \end{aligned}$$

以及

$$\langle q|P = -i \frac{d}{dq} \langle q|. \tag{29}$$

我们可以改写 $|q\rangle\langle p| e^{ipq}$ 为

$$\begin{aligned}
 &\delta(q-Q)\delta(p-P) \\
 &= \frac{1}{\sqrt{2\pi}} |q\rangle\langle p| e^{iPq} \\
 &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dq' e^{-ipq'} |q\rangle\langle q'| e^{iPq}
 \end{aligned}$$

于是有

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dq' e^{-ipq'} |q\rangle\langle q' + q|. \tag{30}$$

$$\begin{aligned}
 &\delta(p-P)\delta(q-Q) \\
 &= \frac{1}{2\pi} \int dq' e^{ipq'} |q + q'\rangle\langle q| \\
 &= \frac{1}{2\pi} \int dq' e^{-ipq'} |q - q'\rangle\langle q|. \tag{31}
 \end{aligned}$$

而介于这两者间的 $\Delta(p, q)$ 在坐标表象中的表达式是

$$\Delta(p, q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy e^{-ipy} \left| q - \frac{1}{2}y \right\rangle \left\langle q + \frac{1}{2}y \right|. \tag{32}$$

所以我们可以组合式(32), (30) 和 (31) 式为一个更一般的形式

$$\begin{aligned}
 &\Omega_k(p, q) \\
 &\equiv \frac{1}{2\pi} \int dy e^{-ipy} \left| q - \frac{k+1}{2}y \right\rangle \left\langle q + \frac{1-k}{2}y \right|. \tag{33}
 \end{aligned}$$

当 $k = -1, 0, 1$, (33) 式分别给出 (30), (32) 和 (31) 式. 而 (33) 式又可进一步改写混合态 $\Omega_k(p, q)$ 为

$$\begin{aligned}
 &\Omega_k(p, q) \\
 &= \frac{1}{2\pi} \int dy e^{-ipy} e^{i\frac{k+1}{2}yP} |q\rangle\langle q| e^{i\frac{1-k}{2}yP} \\
 &= \frac{1}{2\pi} \int dy e^{-ipy} e^{i\frac{k+1}{2}yP} \delta(q-Q) e^{i\frac{1-k}{2}yP} \\
 &= \frac{1}{4\pi^2} \iint_{-\infty}^{\infty} dy du e^{iu(q-Q)+iy(p-P)+i\frac{k}{2}yu}. \tag{34}
 \end{aligned}$$

6 任何算符在混合态表象中表示的求出: 混合态表象的正交性

任何算符可以用它做展开, 所以求它形成表象函数 $h(q, p)$.

由于

$$\begin{aligned}
 &\langle q'' | \Omega_k(p, q) | q' \rangle \\
 &= \frac{1}{2\pi} \int dy e^{-ipy} \\
 &\quad \times \left\langle q'' \left| q - \frac{k+1}{2}y \right\rangle \left\langle q + \frac{1-k}{2}y \right| q' \right\rangle \\
 &= \delta(q-w) e^{ip(q''-q')}, \tag{35}
 \end{aligned}$$

其中

$$w = \frac{1}{2}(q'' + q') - \frac{k}{2}(q'' - q'). \tag{36}$$

结合 (10) 式就有

$$\begin{aligned} & \langle q'' | H | q' \rangle \\ &= \int dq dp \langle q'' | \Omega_k(p, q) | q' \rangle h_k(p, q) \\ &= \int dq dp \delta(q - w) e^{ip(q'' - q')} h_k(p, q) \\ &= \int dp e^{ip(q'' - q')} h_k(p, w), \end{aligned} \quad (37)$$

故

$$\begin{aligned} & h_k\left(p, \frac{1}{2}(q'' + q') - \frac{k}{2}(q'' - q')\right) \\ &= \int dp e^{-ip(q'' - q')} \langle q'' | H | q' \rangle. \end{aligned} \quad (38)$$

让

$$y = q'' - q', \quad q = \frac{1}{2}(q'' + q') - \frac{k}{2}(q'' - q'), \quad (39)$$

(38) 式变成

$$\begin{aligned} & h_k(p, q) \\ &= \int dp e^{-ipy} \left\langle q + \frac{k+1}{2}y \middle| H \middle| q - \frac{1-k}{2}y \right\rangle \\ &= \text{tr} \left[\int dp e^{-ipy} \left| q - \frac{1-k}{2}y \right\rangle \right. \\ & \quad \left. \times \left\langle q + \frac{k+1}{2}y \middle| H \right\rangle \right]. \end{aligned} \quad (40)$$

比较 (33) 式和 (40) 式看出

$$h_k(p, q) = 2\pi \text{tr}[\Omega_{-k}(p, q)H], \quad (41)$$

所以

$$\text{tr}[\Omega_k(p, q)\Omega_{-k}(p', q')] = \frac{1}{2\pi} \delta(q' - q)\delta(p' - p). \quad (42)$$

这就是例混合态表象的正交性. 如现在我们考察算符

$$\sum_{l=0}^{\infty} \binom{m}{l} \left(\frac{1-k}{2}Q\right)^l P^r \left(\frac{1+k}{2}Q\right)^{m-l}, \quad (43)$$

在混合态表象中的表示, 用 (41) 式得到

$$\begin{aligned} & 2\pi \text{tr} \left[\sum_{l=0}^{\infty} \binom{m}{l} \left(\frac{1-k}{2}Q\right)^l P^r \left(\frac{1+k}{2}Q\right)^{m-l} \right. \\ & \quad \left. \times \int dv e^{-ipv} \left| q - \frac{-k+1}{2}y \right\rangle \left\langle q + \frac{1+k}{2}y \right| \right] \\ &= 2\pi \sum_{l=0}^{\infty} \binom{m}{l} \int dv e^{-ipv} \left\langle q + \frac{1+k}{2}y \middle| \left(\frac{1-k}{2}Q\right)^l \right. \\ & \quad \left. \times P^r \left(\frac{1+k}{2}Q\right)^{m-l} \middle| q - \frac{-k+1}{2}y \right\rangle \end{aligned}$$

$$\begin{aligned} &= 2\pi \sum_{l=0}^{\infty} \binom{m}{l} \int dv e^{-ipv} \left[\frac{1-k}{2} \left(q + \frac{1+k}{2}y \right) \right]^l \\ & \quad \times \left[\frac{1+k}{2} \left(q - \frac{-k+1}{2}y \right) \right]^{m-l} \\ & \quad \times \left\langle q + \frac{1+k}{2}y \middle| P^r \middle| q - \frac{-k+1}{2}y \right\rangle \\ &= 2\pi q^m \int dv e^{-ipv} \left\langle q + \frac{1+k}{2}y \middle| P^r \middle| q - \frac{-k+1}{2}y \right\rangle \\ &= q^m p^r. \end{aligned} \quad (44)$$

又如求压缩算符 $\int_{-\infty}^{\infty} \frac{dq'}{\sqrt{\mu}} |q'/\mu\rangle \langle q'| \equiv S_1$ 在混合态表象中的表示,

$$\begin{aligned} & h_k(p, q) \\ &= 2\pi \text{tr}[\Omega_{-k}(p, q)S_1] \\ &= 1/\sqrt{\mu} \text{tr} \left[\int dy e^{-ipy} \left| q - \frac{1-k}{2}y \right\rangle \right. \\ & \quad \left. \times \left\langle q + \frac{1+k}{2}y \middle| \int_{-\infty}^{\infty} dq' |q'/\mu\rangle \langle q'| \right] \right] \\ &= 1/\sqrt{\mu} \int dy e^{-ipy} \left\langle q + \frac{1+k}{2}y \middle| \right. \\ & \quad \left. \times \int_{-\infty}^{\infty} dq' |q'/\mu\rangle \langle q' \middle| q - \frac{1-k}{2}y \right\rangle \\ &= 1/\sqrt{\mu} \int dy e^{-ipy} \int_{-\infty}^{\infty} dq' \\ & \quad \times \delta\left(q + \frac{1+k}{2}y - q'/\mu\right) \\ & \quad \times \delta\left(q' - q + \frac{1-k}{2}y\right) \\ &= 1/\sqrt{\mu} \int dy e^{-ipy} \delta\left(q + \frac{1+k}{2}y - \frac{q - \frac{1-k}{2}y}{\mu}\right) \\ &= 2\sqrt{\mu} \int dy e^{-ipy} \\ & \quad \times \delta[(y - 2q + 2q\mu + y\mu - ky + ky\mu)] \\ &= \frac{2\sqrt{\mu}}{1 + \mu + k\mu - k} \int dy e^{-ipy} \\ & \quad \times \delta\left[y + \frac{2q\mu - 2q}{1 + \mu + k\mu - k}\right] \\ &= \frac{2\sqrt{\mu}}{1 + \mu + k\mu - k} e^{ip \frac{2q\mu - 2q}{1 + \mu + k\mu - k}}. \end{aligned} \quad (45)$$

当 $k = 1$ 为 \mathfrak{P} -排序

$$S_1 = \frac{1}{\sqrt{\mu}} \mathfrak{P} e^{iPQ \frac{\mu-1}{\mu}}. \quad (46)$$

当 $k = -1$ 为 \mathfrak{Q} -排序

$$S_1 = \sqrt{\mu} \mathfrak{Q} e^{iPQ(\mu-1)}. \quad (47)$$

当 $k = 0$, Weyl-排序

$$S_1 = \frac{2\sqrt{\mu}}{1+\mu} e^{i2PQ\frac{\mu-1}{1+\mu}}. \quad (48)$$

7 结 论

我们已从算符的合理排序和概率统计的正态分布思想出发, 提出了量子力学混合态表象, 证明了其完备性和正交性. 混合态表象的优点是可以反映算符的多种表示和相应的排序规则.

附 录

用正规乘积算符内积分技术我们直接对式 (34) 积分,

$$\begin{aligned} & \Omega_k(p, q) \\ &= \frac{1}{4\pi^2} : \iint_{-\infty}^{\infty} dy du \\ & \quad \times e^{-\frac{1}{4}(y^2+u^2)+iu(q-Q)+iy(p-P)+i\frac{k}{2}yu} : \\ &= \frac{1}{2\pi\sqrt{\pi}} : \int du e^{-\frac{1}{4}u^2+iu(q-Q)-(p-P+\frac{k}{2}u)^2} : \\ &= \frac{1}{2\pi\sqrt{\pi}} : \int du \\ & \quad \times e^{-\frac{1}{4}u^2(1+k^2)+iu[q-Q+ik(p-P)]-(p-P)^2} : \\ &= \frac{1}{\pi\sqrt{(1+k^2)}} : \exp\left\{-\frac{(q-Q)^2}{1+k^2}-\frac{2ik}{1+k^2}\right. \\ & \quad \left.\times (q-Q)(p-P)-\frac{(p-P)^2}{1+k^2}\right\} :, \quad (A1) \end{aligned}$$

发现它恰好是数理统计学中的二维正态分布形式^[10].

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Quantum mechanics mixed state representation*

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(Received 18 April 2014; revised manuscript received 26 May 2014)

Abstract

In the previous studies and literatures, quantum mechanics representations are a pure state representation, while in this paper beginning with reasonable ordering of operators in quantum mechanics and the normal distribution thought in probability statistics, we propose the concept of quantum mechanics mixed state representation firstly, and prove its completeness and orthogonality. The advantages of mixed state representation is that it can reflect a variety of expression of quantum mechanics operators and the corresponding operators ordering rules.

Keywords: quantum mechanics mixed state representation, quantum mechanics pure state representation, ordering rules, IWOP technique

PACS: 03.65.-w, 42.50.-p

DOI: [10.7498/aps.63.190302](https://doi.org/10.7498/aps.63.190302)

* Project supported by the National Natural Science Foundation of China (Grant Nos. 11175113, 11275123).

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