

III. 连续谱本征函数的“归一化”

A. 连续谱本征函数“归一化”

1. 本征函数，本征谱

φ_n A_n (取分立值) φ_λ λ (取连续值)

2. 任一波函数可按其展开

$$\psi(\mathbf{x}) = \sum_m c_m \varphi_m(\mathbf{x}) \quad \psi(\mathbf{x}) = \int c_{\lambda'} \varphi_{\lambda'} d\lambda'$$



$$c_n = \int \varphi_n^* \psi dx$$

(φ_n 已归一化)

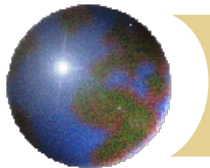
$$c_\lambda = \int \varphi_\lambda^* \psi dx$$

(φ_λ 已归一化)

3. 连续谱本征函数“归一化”

$$c_n = \sum_m c_m \int \varphi_n^* \varphi_m dx \quad \int \varphi_n^* \varphi_m dx = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$$

$$c_\lambda = \int c_{\lambda'} \left(\int \varphi_\lambda^* \varphi_{\lambda'} dx \right) d\lambda'$$



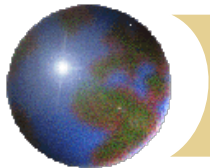
$$\int \varphi_{\lambda}^* \varphi_{\lambda'} dx = \begin{cases} 0 & \lambda' \neq \lambda \\ \infty & \lambda' = \lambda \end{cases}$$

所以， $\int \varphi_{\lambda}^* \varphi_{\lambda'} dx$ 是一“奇异函数”。

我们引入一个奇异函数，即 $\delta(\mathbf{x})$ ，
其定义

$$\delta(\mathbf{x} - \mathbf{x}_0) = \begin{cases} 0 & \mathbf{x} - \mathbf{x}_0 \neq 0 \\ \infty & \mathbf{x} - \mathbf{x}_0 = 0 \end{cases}$$

以及



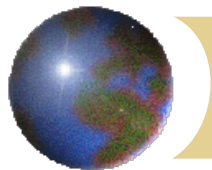
$$\int_a^b f(x)\delta(x - x_0)dx = \begin{cases} f(x_0) & a < x_0 < b \\ 0 & (a, b) \notin x_0 \end{cases}$$

因此，如

$$\int \varphi_\lambda^* \varphi_{\lambda'} dx = \delta(\lambda - \lambda'),$$

则

$$\int c_{\lambda'} (\int \varphi_\lambda^* \varphi_{\lambda'} dx) d\lambda' = \int c_{\lambda'} \delta(\lambda - \lambda') d\lambda' = c_\lambda$$



这就保证获得我们所需结果。

所以，连续谱“归一化”的本征函数 φ_λ 应使其有

$$(\varphi_\lambda, \varphi_{\lambda'}) = \delta(\lambda - \lambda')$$

例1 求“正交归一”的动量本征函数

设： $\psi(x)$ 是平方可积，即可进行傅里叶展

开

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int F(k') e^{ik'x} dk'$$



$$F(\mathbf{k}) = \frac{1}{\sqrt{2\pi}} \int e^{-i\mathbf{k}\mathbf{x}} \psi(\mathbf{x}) d\mathbf{x}$$

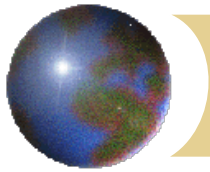
$$= \frac{1}{2\pi} \int F(\mathbf{k}') e^{i(\mathbf{k}' - \mathbf{k})\mathbf{x}} d\mathbf{x} d\mathbf{k}'$$

于是应有

$$F(\mathbf{k}) = \int F(\mathbf{k}') \delta(\mathbf{k}' - \mathbf{k}) d\mathbf{k}'$$

所以，

$$\frac{1}{2\pi} \int e^{i(\mathbf{k}' - \mathbf{k})\mathbf{x}} d\mathbf{x} = \delta(\mathbf{k}' - \mathbf{k})$$



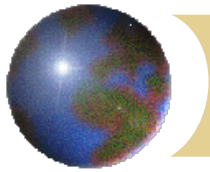
“正交归一”的动量本征函数为

$$\varphi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

事实上，由于物理波函数在无穷远为 0

$$(u_k, u_{k'}) = \frac{1}{2\pi} \lim_{\varepsilon \rightarrow 0^+} \int e^{i(k'-k)x - \varepsilon|x|} dx$$

$$= \frac{1}{2\pi} \lim_{\varepsilon \rightarrow 0^+} \left[\int_0^{+\infty} e^{i(k'-k)x - \varepsilon x} dx + \int_{-\infty}^0 e^{i(k'-k)x + \varepsilon x} dx \right]$$

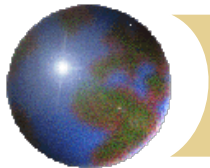


$$= \frac{1}{2\pi} \lim_{\varepsilon \rightarrow 0^+} \left[\frac{-1}{i(k' - k) - \varepsilon} + \frac{1}{i(k' - k) + \varepsilon} \right]$$

$$= \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \left[\frac{\varepsilon}{(k' - k)^2 + \varepsilon^2} \right]$$

$$= \delta(k' - k)$$

于是有
$$\mathbf{u}_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{2\pi}} \lim_{\varepsilon \rightarrow 0^+} e^{i\mathbf{k}\mathbf{x} - \varepsilon|\mathbf{x}|/2}$$



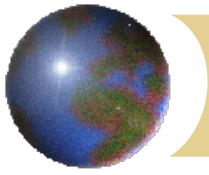
例2 求“正交归一”的坐标本征函数
由坐标本征方程

$$\hat{x}\varphi_{x'}(x) = x'\varphi_{x'}(x)$$

\hat{x} 的“正交归一”的坐标本征函数为

$$\varphi_{x'}(x) = \delta(x - x')$$

它是完备的： $\psi(x) = \int \psi(x')\delta(x' - x)dx'$



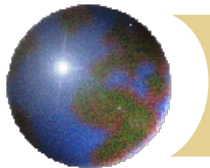
4. 因

$$\bar{\hat{A}} = \sum_{\mathbf{n}} A_{\mathbf{n}} |c_{\mathbf{n}}|^2$$

$|c_{\mathbf{n}}|^2$ 表示在态 $\psi(\mathbf{x})$ 中测量力学量 \hat{A} 取 $A_{\mathbf{n}}$ 的概率。

而由

$$\begin{aligned} \bar{\lambda} &= \int \psi^*(\mathbf{x}) \hat{\lambda} \psi(\mathbf{x}) d\mathbf{x} \\ &= \int \int c_{\lambda}^* \varphi_{\lambda}^* d\lambda \hat{\lambda} \int c_{\lambda'} \varphi_{\lambda'} d\lambda' d\mathbf{x} \end{aligned}$$

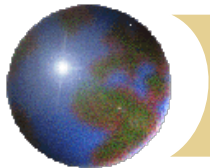


$$= \int c_{\lambda}^* c_{\lambda'} \varphi_{\lambda}^* \varphi_{\lambda'} dx d\lambda d\lambda'$$

$$= \int c_{\lambda}^* c_{\lambda'} \delta(\lambda - \lambda') d\lambda d\lambda'$$

$$= \int \lambda |c_{\lambda}|^2 d\lambda$$

由这可见（如 $\psi(x)$ 已归一化）， $|c_{\lambda}|^2 d\lambda$
为测量 $\hat{\lambda}$ 取值在区域 $\lambda - \lambda + d\lambda$ 中的概率

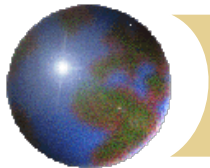


Delta函数性质

详见程老师课件

↑ C. 本征函数的封闭性

已经讨论过厄密算符本征态的正交、归一和完备性，即



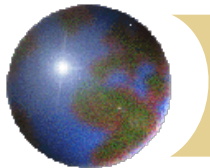
$$(\mathbf{u}_n, \mathbf{u}_m) = \delta_{nm} \quad (\text{正交, 归一})$$

$$\psi = \sum_n c_n u_n \quad (\text{完备})$$

对于连续谱 $(\varphi_\lambda, \varphi_{\lambda'}) = \delta(\lambda - \lambda')$

$$\psi(x) = \int c_\lambda \varphi_\lambda d\lambda$$

下面我们来讨论本征函数的封闭性



$$\psi(\mathbf{x}) = \sum_n c_n u_n(\mathbf{x}) \quad c_n = \int u_n^*(\mathbf{x}') \psi(\mathbf{x}') d\mathbf{x}'$$

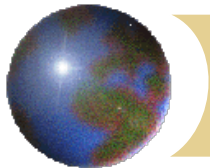
u_n 已归一化

所以

$$\psi(\mathbf{x}) = \int \left(\sum_n u_n(\mathbf{x}) u_n^*(\mathbf{x}') \right) \psi(\mathbf{x}') d\mathbf{x}'$$

由此可见，

$$\sum_n u_n(\mathbf{x}) u_n^*(\mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$$



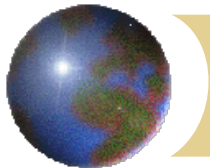
上述表示式称为本征函数的封闭性，
它表明本征函数组可构成一 δ 函数

例1 \hat{L}_z 的本征函数

$$\psi_m = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad m = 0, \pm 1, \pm 2, \pm 3 \dots$$

有
$$\sum_m \psi_m(\phi) \psi_m^*(\phi') = \delta(\phi - \phi')$$

即
$$\frac{1}{2\pi} \sum_m e^{im(\phi - \phi')} = \delta(\phi - \phi')$$



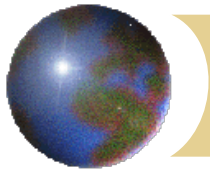
另一形式：
$$\frac{1}{2l} \sum_m e^{i\frac{\pi}{l}(x-x')m} = \delta(x-x') \quad \phi = \frac{\pi}{l}x$$

例2 \hat{p}_x 的本征函数

$$\psi_{p_x} = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_x x / \hbar}$$

$$\int \psi_{p_x}(x) \psi_{p_x}^*(x') dp_x = \delta(x-x')$$

$$\frac{1}{2\pi\hbar} \int e^{ip_x(x-x')/\hbar} dp_x = \delta(x-x')$$



1. 封闭性是正交、归一的本征函数完备性的充分必要条件。

若

φ_n 是完备的 $\xrightarrow{\text{必有}}$ 封闭性 (必要条件)

有封闭性 $\xrightarrow{\text{则是}}$ 完备的 (充分条件)

a. 必要条件已证过

b. 充分条件:



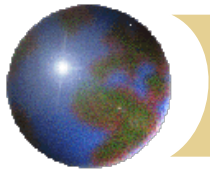
有封闭性:

$$\sum_m \varphi_m(\mathbf{x}) \varphi_m^*(\mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$$

$$\psi(\mathbf{x}) = \int \delta(\mathbf{x} - \mathbf{x}') \psi(\mathbf{x}') d\mathbf{x}'$$

$$= \int \sum_m \varphi_m(\mathbf{x}) \varphi_m^*(\mathbf{x}') \psi(\mathbf{x}') d\mathbf{x}'$$

$$= \sum_m c_m \varphi_m(\mathbf{x})$$

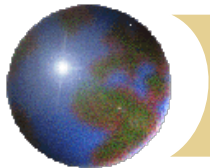


2. 本征函数的封闭性也可看作 $\delta(\mathbf{x})$ 函数按本征函数展开，而展开系数恰为本征函数的复共轭。

$$\delta(\mathbf{x} - \mathbf{x}') = \sum_n c_n^{\mathbf{x}'} \varphi_n(\mathbf{x})$$

$$c_n^{\mathbf{x}'} = \int \varphi_n^*(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') d\mathbf{x} = \varphi_n^*(\mathbf{x}')$$

$$\delta(\mathbf{x} - \mathbf{x}') = \sum_n \varphi_n(\mathbf{x}) \varphi_n^*(\mathbf{x}')$$

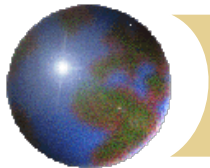


IV . 算符的共同本征函数

一次测量有一“涨落”

$$\Delta A = \sqrt{\overline{\Delta \hat{A}^2}} = \sqrt{(\psi, \Delta \hat{A}^2 \psi)} = \sqrt{(\psi, (\hat{A} - \overline{\hat{A}})^2 \psi)}$$

两个算符，在一个态中，一般都有涨落， $\overline{\Delta \hat{A}^2}$ ， $\overline{\Delta \hat{B}^2}$ 不同时为零。在什么条件下， \hat{A} ， \hat{B} 有共同本征函数组



↑

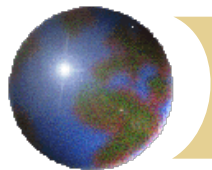
A. 算符“涨落”之间的关系

1. Schwartz不等式

如果 ψ_1, ψ_2 是任意两个平方可积的波函数，则

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

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



而

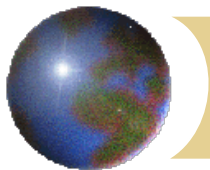
$$(\Psi_3, \Psi_3) = \left(\Psi_2 - \Psi_1 \frac{(\Psi_1, \Psi_2)}{(\Psi_1, \Psi_1)}, \Psi_2 - \Psi_1 \frac{(\Psi_1, \Psi_2)}{(\Psi_1, \Psi_1)} \right) \geq 0$$

得

$$\begin{aligned} & (\Psi_2, \Psi_2) - (\Psi_2, \Psi_1) \frac{(\Psi_1, \Psi_2)}{(\Psi_1, \Psi_1)} - \frac{(\Psi_1, \Psi_2)^*}{(\Psi_1, \Psi_1)} (\Psi_1, \Psi_2) \\ & + \left(\frac{(\Psi_1, \Psi_2)^*}{(\Psi_1, \Psi_1)} \frac{(\Psi_1, \Psi_2)}{(\Psi_1, \Psi_1)} (\Psi_1, \Psi_1) \right) \geq 0 \end{aligned}$$

从而证得：

$$(\Psi_1, \Psi_1) \cdot (\Psi_2, \Psi_2) \geq |(\Psi_2, \Psi_1)|^2$$



2. 算符“涨落”之间的关系—不确定

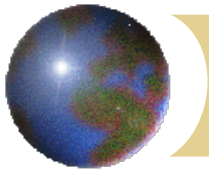
关系：

$$\overline{\Delta\hat{A}^2} \cdot \overline{\Delta\hat{B}^2} \geq \frac{1}{4} \left| \int \psi^* [\hat{A}, \hat{B}] \psi dx \right|^2$$

$$\Delta A \cdot \Delta B \geq \frac{\overline{i[\hat{A}, \hat{B}]}}{2}$$

证明： 如令

$$\psi_1 = (\hat{A} - \bar{A})\psi \quad \psi_2 = (\hat{B} - \bar{B})\psi$$



$$\begin{aligned} & |(\psi_1, \psi_2)|^2 \\ & \geq \left| \frac{1}{2i} [(\psi_1, \psi_2) - (\psi_2, \psi_1)] \right|^2 \\ & = \left| \frac{1}{2i} [((\hat{A} - \bar{A})\psi, (\hat{B} - \bar{B})\psi) - ((\hat{B} - \bar{B})\psi, (\hat{A} - \bar{A})\psi)] \right|^2 \\ & = \left| \frac{1}{2i} [(\psi, (\hat{A} - \bar{A})(\hat{B} - \bar{B})\psi) - (\psi, (\hat{B} - \bar{B})(\hat{A} - \bar{A})\psi)] \right|^2 \\ & = \left| \frac{1}{2i} [(\psi, (\hat{A}\hat{B} - \hat{A}\bar{B} - \bar{A}\hat{B} + \bar{A}\bar{B})\psi) - (\psi, (\hat{B}\hat{A} - \bar{B}\hat{A} - \hat{B}\bar{A} + \bar{B}\bar{A})\psi)] \right|^2 \end{aligned}$$



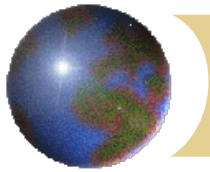
$$= \left| \frac{1}{2i} [(\psi, (\hat{A}\hat{B})\psi) - (\psi, (\hat{B}\hat{A})\psi)] \right|$$
$$= \left| \frac{1}{2i} (\psi, [\hat{A}, \hat{B}]\psi) \right|^2$$

由

$$(\psi_1, \psi_1) \cdot (\psi_2, \psi_2) \geq \left| \frac{1}{2i} (\psi, [\hat{A}, \hat{B}]\psi) \right|^2$$

$$\overline{\Delta\hat{A}^2} \cdot \overline{\Delta\hat{B}^2} \geq \frac{1}{4} \left| \int \psi [\hat{A}, \hat{B}] \psi dx \right|^2$$

$$\Delta A \cdot \Delta B \geq \frac{\boxed{i[\hat{A}, \hat{B}]}}{2}$$



例1 $\hat{A} = x$, $\hat{B} = \hat{p}_x$

$$[\hat{A}, \hat{B}] = [x, \hat{p}_x] = i\hbar$$

由于是一常数，所以在任何态下平均都不可能为零。我们有

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}$$

这即为海森伯（Heisenberg）的不确定关系的严格证明。



例2

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

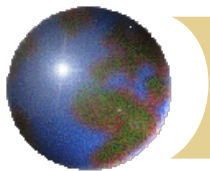
但在态 $Y_{00} = \frac{1}{\sqrt{4\pi}}$ 时

$$\overline{[\hat{L}_x, \hat{L}_y]} = \overline{i\hbar \hat{L}_z} = 0 \quad \overline{\Delta \hat{L}_x^2} \cdot \overline{\Delta \hat{L}_y^2} = 0$$

即

$$\overline{\Delta \hat{L}_x^2} = \overline{\Delta \hat{L}_y^2} = 0$$

但这仅是某一特殊态。



B. 算符的共同本征函数组

定理 1. 如果两个力学量相应的算符有一组正交，归一，完备的共同本征函数组，则算符 \hat{A} ， \hat{B} 必对易， $[\hat{A}, \hat{B}] = 0$ 。

证：

设 $V_{nm}^{(t)}(\mathbf{x})$ 为算符 \hat{A} ， \hat{B} 的共同本征函数组。

$$\hat{A}V_{nm}^{(t)} = A_n V_{nm}^{(t)} \quad \hat{B}V_{nm}^{(t)} = B_m V_{nm}^{(t)}$$



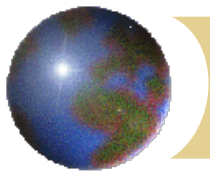
对于任一波函数 $\psi(\mathbf{x})$ 都有

$$\psi(\mathbf{x}) = \sum_{n,m,t} C_t^{nm} \mathbf{V}_{nm}^{(t)}$$

于是

$$[\hat{A}, \hat{B}] \psi(\mathbf{x}) = \sum_{n,m,t} C_t^{nm} [\hat{A}, \hat{B}] \mathbf{V}_{nm}^{(t)}$$

$$= \sum_{n,m,t} C_t^{nm} [A_n, B_m] \mathbf{V}_{nm}^{(t)} = 0$$

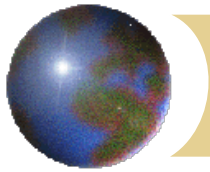


因 $\psi(\mathbf{x})$ 是任意的，所以， $[\hat{A}, \hat{B}] = 0$ ，
即 \hat{A} ， \hat{B} 对易。

定理 2：如果两力学量所相应算符对
易， $[\hat{A}, \hat{B}] = 0$ ，则它们有共同的正交，归
一和完备的本征函数组。

证：设 $\varphi_n^{(s)}$ 是 \hat{A} 的本征函数组。

$$\hat{A}\varphi_n^{(s)} = A_n\varphi_n^{(s)}$$



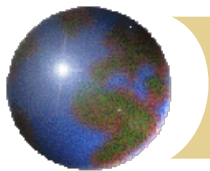
如 $s = 1$ ，即不简并，于是

$$\hat{A}\hat{B}\varphi_n = \hat{B}\hat{A}\varphi_n = A_n\hat{B}\varphi_n$$

当 \hat{A} 的本征函数不简并时，就有

$$\hat{B}\varphi_n = B_n\varphi_n$$

则 $\{\varphi_n\}$ 是它们的共同完备的本征函数组。



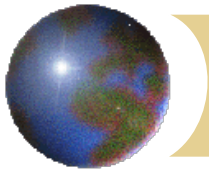
当 $s > 1$ ，即有简并。无妨设 \hat{B} 的本征函数组为 $\mathbf{u}_m^{(r)}$ （这也是一完备组）。

$$\hat{B}\mathbf{u}_m^{(r)} = b_m \mathbf{u}_m^{(r)}$$

将 $\varphi_n^{(s)}$ 展开

$$\varphi_n^{(s)} = \sum_{r,m} c_{nr}^{(s)m} \mathbf{u}_m^{(r)}$$

$$\hat{A}\varphi_n^{(s)} = A_n \varphi_n^{(s)}$$



即

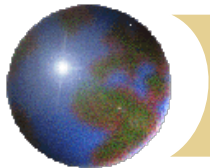
$$\hat{\mathbf{A}} \sum_{m,r} \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)} = \mathbf{A}_n \sum_{m,r} \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)}$$

$$\sum_m \hat{\mathbf{A}} \left(\sum_r \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)} \right) = \sum_m \mathbf{A}_n \left(\sum_r \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)} \right)$$

而

$$\hat{\mathbf{B}} \left(\hat{\mathbf{A}} \sum_r \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)} \right) = \hat{\mathbf{A}} \hat{\mathbf{B}} \sum_r \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)}$$

$$= \mathbf{b}_m \left(\hat{\mathbf{A}} \sum_r \mathbf{c}_{nr}^{(s)m} \mathbf{u}_m^{(r)} \right)$$



$$\hat{\mathbf{B}} \mathbf{A}_n \sum_{\mathbf{r}} (\mathbf{c}_{\mathbf{nr}}^{(s)m} \mathbf{u}_{\mathbf{m}}^{(r)}) = \mathbf{b}_m \mathbf{A}_n \sum_{\mathbf{r}} (\mathbf{c}_{\mathbf{nr}}^{(s)m} \mathbf{u}_{\mathbf{m}}^{(r)})$$

所以

$$\hat{\mathbf{A}} \sum_{\mathbf{r}} \mathbf{c}_{\mathbf{nr}}^{(s)m} \mathbf{u}_{\mathbf{m}}^{(r)} = \mathbf{A}_n \sum_{\mathbf{r}} \mathbf{c}_{\mathbf{nr}}^{(s)m} \mathbf{u}_{\mathbf{m}}^{(r)}$$

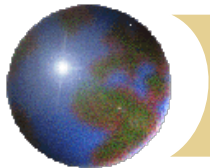
这表明， $\sum_{\mathbf{r}} \mathbf{c}_{\mathbf{nr}}^{(s)m} \mathbf{u}_{\mathbf{m}}^{(r)}$

是算符 $\hat{\mathbf{A}}$ ， $\hat{\mathbf{B}}$ 的本征值为 \mathbf{A}_n ， \mathbf{B}_m 的共同本征函数。对任一波函数有



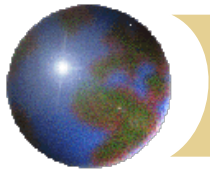
$$\begin{aligned}\psi &= \sum_{n,s} d_s^n \varphi_n^{(s)} \\ &= \sum_{n,s} d_s^n \sum_{m,r} c_{nr}^{(s)m} u_m^{(r)} \\ &= \sum_{n,s,m} d_s^n \left(\sum_r c_{nr}^{(s)m} u_m^{(r)} \right)\end{aligned}$$

所以它们是完备的（对所有 n, m, s 的集合）。



即，两力学量所相应算符对易， $[\hat{A}, \hat{B}] = 0$
则它们有共同的正交，归一和完备的
本征函数组

4.10 **4.11**

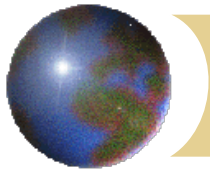


同理

$$\mathbf{V}_a^{(b_2)} = \mathbf{c}_1^{(1)} \left[\mathbf{u}_a^{(1)} + \frac{(\mathbf{b}_2 - \mathbf{b}_{11})}{\mathbf{b}_{12}} \mathbf{u}_a^{(2)} \right]$$

\hat{A}, \hat{B} 的本征值就唯一地决定波函数 $\mathbf{V}_a^{(b_i)}$ 。
它们的共同本征态没有一个是简并的。

力学量完全集：设力学量 $\hat{A}, \hat{B}, \hat{C} \dots$ 彼此对易；它们的共同本征函数 $u_{abc} \dots$ 是不简并的，也就是说，本征值 $a, b, c \dots$ 仅对应一个独立的本征函数，则称这一组力学量为力学量完全集。



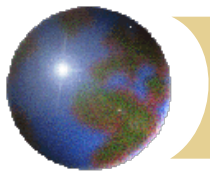
所以，以后要描述一个体系所处的态时，我们首先集中注意力去寻找一组独立的完全集，以给出特解，然后得到通解。

有了力学量完全集， $u_{nabc\dots}$ ，则可得

$$\psi(\underline{r}, t) = \sum_{n,a,b,c\dots} c_{nabc\dots} u_{nabc\dots} e^{-iE_n t / \hbar}$$

$$c_{nabc\dots} = \int u_{nabc\dots}^*(\underline{r}) \psi(\underline{r}, 0) d\underline{r}$$

\hat{L}^2, \hat{L}_z 完全集相应的本征函数组为 $Y_{lm}(\theta, \phi)$



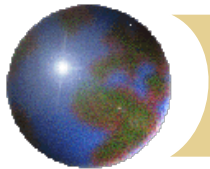
↑ C. 角动量的共同本征函数组—球谐函数
因 $[\hat{L}^2, \hat{L}_z] = 0$ ， 它们有共同本征函数组

1. 本征值:

设: u_{lm} 是它们的共同本征函数, 则

$$\hat{L}^2 u_{lm} = \eta_l \hbar^2 u_{lm}$$

$$\hat{L}_z u_{lm} = m \hbar u_{lm}$$



$$\odot \quad (\hat{L}^2 - \hat{L}_z^2) \mathbf{u}_{lm} = (\eta_l - m^2) \hbar^2 \mathbf{u}_{lm}$$

$$\hat{L}^2 - \hat{L}_z^2 = \hat{L}_x^2 + \hat{L}_y^2$$

$$\eta_l \geq m^2 \quad |m| \leq \eta_l^{1/2}$$

固定 η_l 时, m 有上, 下限。

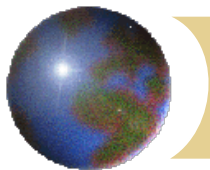
$$\odot \quad [\hat{L}_z, \hat{L}_-] = \hat{L}_z \hat{L}_- - \hat{L}_- \hat{L}_z = -\hbar \hat{L}_-$$

其中 $\hat{L}_- = \hat{L}_x - i\hat{L}_y$



$$\begin{aligned}[\hat{\mathbf{L}}_z, \hat{\mathbf{L}}_-] &= \hat{\mathbf{L}}_z, \hat{\mathbf{L}}_- - \mathbf{L}_- \hat{\mathbf{L}}_z \\ &= \hat{\mathbf{L}}_z \hat{\mathbf{L}}_x - i \hat{\mathbf{L}}_z \hat{\mathbf{L}}_y - \mathbf{L}_x \hat{\mathbf{L}}_z + i \mathbf{L}_y \hat{\mathbf{L}}_z \\ &= i \hbar \hat{\mathbf{L}}_y + i \cdot i \hbar \mathbf{L}_x = -\hbar \hat{\mathbf{L}}_-\end{aligned}$$

$$\begin{aligned}[\hat{\mathbf{L}}_z, \hat{\mathbf{L}}_+] &= \hat{\mathbf{L}}_z, \hat{\mathbf{L}}_+ - \mathbf{L}_+ \hat{\mathbf{L}}_z \\ &= \hat{\mathbf{L}}_z \hat{\mathbf{L}}_x + i \hat{\mathbf{L}}_z \hat{\mathbf{L}}_y - \mathbf{L}_x \hat{\mathbf{L}}_z - i \mathbf{L}_y \hat{\mathbf{L}}_z \\ &= i \hbar \hat{\mathbf{L}}_y - i \cdot i \hbar \mathbf{L}_x = \hbar \hat{\mathbf{L}}_+\end{aligned}$$



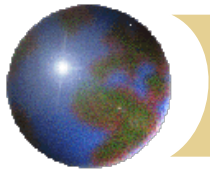
$$\hat{L}_z \hat{L}_- \mathbf{u}_{lm} = \hat{L}_- (\hat{L}_z - \hbar) \mathbf{u}_{lm} = (m - 1) \hbar \hat{L}_- \mathbf{u}_{lm}$$

$$\begin{array}{cccc} \mathbf{u}_{lm} & \hat{L}_- \mathbf{u}_{lm} & (\hat{L}_-)^2 \mathbf{u}_{lm} & (\hat{L}_-)^3 \mathbf{u}_{lm} \cdots \\ m\hbar & (m-1)\hbar & (m-2)\hbar & (m-3)\hbar \cdots \end{array}$$

称 \hat{L}_- 为降算符。

类似地，由 $[\hat{L}_z, \hat{L}_+] = \hbar \hat{L}_+$ 得

$$\hat{L}_z \hat{L}_+ \mathbf{u}_{lm} = \hat{L}_+ (\hat{L}_z + \hbar) \mathbf{u}_{lm} = (m + 1) \hbar \hat{L}_+ \mathbf{u}_{lm}$$



$$\begin{array}{cccc} \mathbf{u}_{lm} & \hat{L}_+ \mathbf{u}_{lm} & (\hat{L}_+)^2 \mathbf{u}_{lm} & (\hat{L}_+)^3 \mathbf{u}_{lm} \cdots \\ m\hbar & (m+1)\hbar & (m+2)\hbar & (m+3)\hbar \cdots \end{array}$$

称 \hat{L}_+ 为升算符 (对 \hat{L}_z 而言)。

⊙ 由于 $|m| \leq \eta_1^{1/2}$, η_1 固定时, m 有上、下限。若设 m_+ 为上限, m_- 为下限, 则

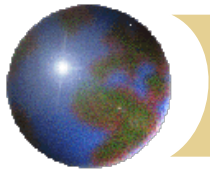
$$\hat{L}_+ \mathbf{u}_{lm_+} = 0 \quad \hat{L}_- \mathbf{u}_{lm_-} = 0$$



$$\hat{L}_- \hat{L}_+ u_{lm_+} = 0 \quad \hat{L}_+ \hat{L}_- u_{lm_-} = 0$$

$$\begin{aligned} \hat{L}_- \hat{L}_+ &= (\hat{L}_x - i\hat{L}_y)(\hat{L}_x + i\hat{L}_y) \\ &= \hat{L}_x^2 + \hat{L}_y^2 + i\hat{L}_x \hat{L}_y - i\hat{L}_y \hat{L}_x \\ &= \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z \end{aligned}$$

$$\begin{aligned} \hat{L}_+ \hat{L}_- &= (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y) \\ &= \hat{L}_x^2 + \hat{L}_y^2 - i\hat{L}_x \hat{L}_y + i\hat{L}_y \hat{L}_x \end{aligned}$$



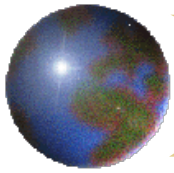
$$\bullet \quad = \hat{\mathbf{L}}^2 - \hat{\mathbf{L}}_z^2 + \hbar \hat{\mathbf{L}}_z$$

$$(\hat{\mathbf{L}}^2 - \hat{\mathbf{L}}_z^2 - \hbar \hat{\mathbf{L}}_z) \mathbf{u}_{l m_+} = (\eta_l - m_+^2 - m_+) \hbar^2 \mathbf{u}_{l m_+} = 0$$

$$(\hat{\mathbf{L}}^2 - \hat{\mathbf{L}}_z^2 + \hbar \hat{\mathbf{L}}_z) \mathbf{u}_{l m_-} = (\eta_l - m_-^2 + m_-) \hbar^2 \mathbf{u}_{l m_-} = 0$$

$$\begin{aligned} \eta_l = m_+ (m_+ + 1) &\Rightarrow m_+ = m_- - 1 \\ \eta_l = m_- (m_- - 1) &\Rightarrow m_+ = -m_- \end{aligned}$$

m_+ 为上限, **m_-** 为下限,



所以，只能取

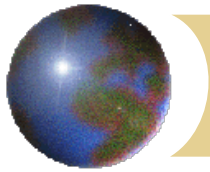
$$m_+ = -m_- = l$$

\hat{L}^2 的本征值可取

$$\eta_l = l(l+1)\hbar^2$$

\hat{L}_z 的本征值可取

$$-l\hbar, (-l+1)\hbar, (-l+2)\hbar, \dots, 0, \dots, (l-2)\hbar, (l-1)\hbar, l\hbar$$



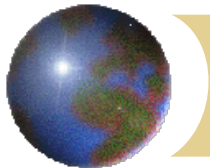
即，取

$$m\hbar$$

$$-l \leq m \leq l \quad l = 0, 1, 2, 3, \dots$$

这表明，**角动量的本征值是量子化的**。它与能量量子化不同在于它并不需要粒子是束缚的。**自由粒子的角动量是量子化的**。

2. 本征函数



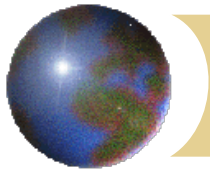
$$-i\hbar \frac{\partial}{\partial \phi} \mathbf{u}_{lm} = m\hbar \mathbf{u}_{lm}$$

于是有解 $\mathbf{u}_{lm(\theta, \phi)} = \mathbf{A}_{lm}(\theta) e^{im\phi}$

○ $\hat{L}_+ = \hbar e^{i\phi} \left(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$, 所以有

$$\hat{L}_+ \mathbf{u}_{ll} = \hat{L}_+ \mathbf{A}_{ll(\theta)} e^{ill} = 0$$

$$e^{i(l+1)\phi} \left(\frac{d}{d\theta} - l \cot \theta \right) \mathbf{A}_{ll}(\theta) = 0$$

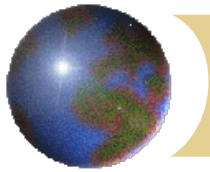


而 $\left(\frac{d}{d\theta} - l \cot \theta \right) = \sin^l \theta \frac{d}{d\theta} \frac{1}{\sin^l \theta}$, 即得

$$\sin^l \theta \frac{d}{d\theta} \frac{1}{\sin^l \theta} A_{ll}(\theta) = 0 \quad A_{ll}(\theta) = c \sin^l \theta$$

⊙ 现求归一化系数

$$c^2 \int_0^\pi \sin^{2l+1} \theta d\theta \int_0^{2\pi} d\phi = 1$$
$$2\pi c^2 (-1)^{2l} \frac{2^{2l+1} (l!)^2}{(2l+1)!} = 1$$



得归一化的本征函数

$$\mathbf{u}_{ll(\theta,\phi)} = (-1)^l \frac{1}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} \sin^l \theta e^{il\phi}$$

$$\odot \quad \mathbf{u}_{lm(\theta,\phi)} \propto \mathbf{c}(\hat{\mathbf{L}}_-)^{l-m} \sin^l \theta e^{im\phi}$$

现先讨论 u_{lm} 的归一化问题，然后给出 u_{lm} 的具体形式。

若 \mathbf{u}_{lm} 是归一化的，则



$$u_{lm-1} \propto \hat{L}_- u_{lm}$$

$$\int (\hat{L}_- u_{lm})^* \hat{L}_- u_{lm} d\Omega$$

$$= \int u_{lm}^* \hat{L}_+ \hat{L}_- u_{lm} d\Omega$$

$$= [l(l+1) - m^2 + m] \hbar^2$$

$$\bullet \odot \quad u_{lm-1} = \frac{1}{\sqrt{(l+m)(l-m+1)\hbar}} \hat{L}_- u_{lm}$$



现求归一化的波函数

$$\hat{L}_- = \hbar e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$$

⊙ $\hat{L}_- u_{ll} = c \hat{L}_- \sin^l \theta e^{il\phi}$

$$= c \hbar e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) \sin^l \theta e^{il\phi}$$

$$= c \hbar \left(-\frac{d}{d\theta} - l \cot \theta \right) \sin^l \theta e^{i(l-1)\phi}$$



$$= -c\hbar \left(\frac{1}{\sin^l \theta} \frac{d}{d\theta} \sin^l \theta \right) \sin^l \theta e^{i(l-1)\phi}$$

所以,

$$\cdot \mathbf{u}_{l-1} = \frac{c}{\sqrt{2l-1}} (-1) \frac{1}{\sin^l \theta} \frac{d}{d\theta} \sin^{2l} \theta e^{i(l-1)\phi}$$

$$\hat{L}_- e^{i(m'+1)\phi} = (-1)\hbar e^{-i\phi} \left(\frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right) e^{i(m'+1)\phi}$$

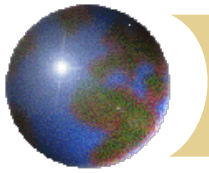
$$= (-1)\hbar e^{im'\phi} \left(\frac{1}{\sin^{m'+1} \theta} \frac{d}{d\theta} \sin^{m'+1} \theta \right)$$



$$\hat{\mathbf{L}}_{-} \mathbf{u}_{l-1} = \frac{\mathbf{c}\hbar}{\sqrt{2l \cdot 1}} (-1)^2 e^{-i\phi} \left(\frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right) \frac{1}{\sin^1 \theta} \frac{\mathbf{d}}{\mathbf{d}\theta} \sin^{2l} \theta e^{i(l-1)\phi}$$

$$= \frac{\mathbf{c}\hbar}{\sqrt{2l \cdot 1}} (-1)^2 e^{i(l-2)\phi} \left(\frac{1}{\sin^{(l-1)} \theta} \frac{\mathbf{d}}{\mathbf{d}\theta} \sin^{(l-1)} \theta \right) \frac{1}{\sin^1 \theta} \frac{\mathbf{d}}{\mathbf{d}\theta} \sin^{2l} \theta$$

$$\mathbf{u}_{l-2} = \frac{\mathbf{c}}{\sqrt{2l \cdot (2l-1) \cdot 1 \cdot 2}} (-1)^2 \frac{1}{\sin^{(l-1)} \theta} \frac{\mathbf{d}}{\mathbf{d}\theta} \frac{1}{\sin \theta} \frac{\mathbf{d}}{\mathbf{d}\theta} \sin^{2l} \theta e^{i(l-2)\phi}$$

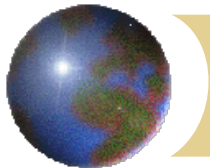


以此类推

$$u_{lm} = \frac{c}{\sqrt{2l \cdot (2l-1) \cdots (l+m+1) \cdot 1 \cdot 2 \cdots (l-m)}} (-1)^{l-m} \frac{1}{\sin^{m+1} \theta}.$$

$$\cdot \overbrace{\frac{d}{d\theta} \frac{1}{\sin \theta} \frac{d}{d\theta} \cdots \frac{1}{\sin \theta} \frac{d}{d\theta}}^{l-m} \sin^{2l} \theta e^{im\phi}$$

$$\cdot = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} \frac{1}{\sin^m \theta} \left(\frac{d}{d \cos \theta} \right)^{l-m} \sin^{2l} \theta e^{im\phi}$$

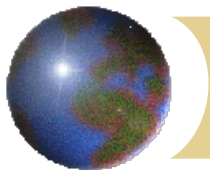


于是得 \hat{L}^2, \hat{L}_z 的共同本征函数组-球谐函数

$$Y_{lm} = (-1)^m \sqrt{\frac{(2l+1)}{4\pi}} \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}$$

$$P_l^m(\cos\theta) = (-1)^{l+m} \frac{1}{2^l l!} \frac{(l+m)!}{(l-m)!} \frac{1}{\sin^m\theta} \left(\frac{d}{d\cos\theta}\right)^{l-m} \sin^{2l}\theta$$

称为连带勒让德函数。



当 l, m 给定，也就是 \hat{L}^2, \hat{L}_z 的本征值
给定，那就唯一地确定了本征函数 $Y_{lm}(\theta, \phi)$

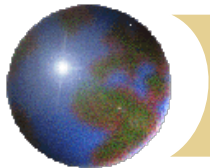
其性质：

a. 正交归一

$$\int Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi) d\Omega = \delta_{ll'} \delta_{mm'}$$

b. 封闭性

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} Y_{lm}(\theta, \phi) Y_{lm}^*(\theta', \phi') = \delta(\Omega - \Omega') = \frac{1}{\sin \theta} \delta(\theta - \theta') \delta(\phi - \phi')$$

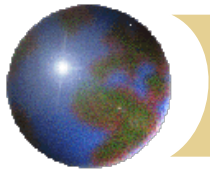


c. 因

$$P_l^{-m}(\cos \theta) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\cos \theta) \quad m \geq 0$$

所以，

$$\begin{aligned} Y_{l-m} &= (-1)^{-m} \sqrt{\frac{(2l+1)}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} P_l^{-m}(\cos \theta) e^{-im\phi} \\ &= \sqrt{\frac{(2l+1)}{4\pi}} \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) e^{-im\phi} \end{aligned}$$



因此, $Y_{l-m} = (-1)^m Y_{lm}^*$

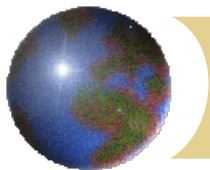
d. Y_{lm} 宇称 $(-1)^l$

• $\underline{r} \rightarrow -\underline{r}$, 即 $\theta \rightarrow \pi - \theta$ $\phi \rightarrow \pi + \phi$
 $(-1)^{l-m}$ $(-1)^m$

e. 递推关系

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

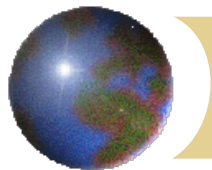
$$\hat{L}_+ Y_{lm} = \sqrt{(l-m)(l+m+1)} \hbar Y_{lm+1}$$



↑ D. 力学量的完全集

在量子力学中，是**确定体系所处的状态**而不是轨道。是确定对体系测量某力学量的可能值及相应概率。所以，若能充分确定状态，则认为**是完全描述了**。但是，如何才能将状态描述完全确定呢？

设： **\hat{A}, \hat{B}** 是力学量所对应的算符，并且对易。显然，如 **$u_a(\mathbf{x})$** 是 \hat{A} 的本征函数



，则 $\hat{B}u_a$ 也是 \hat{A} 的本征函数。

★ \hat{A} 的本征函数不简并，则

$$\hat{B}u_a = bu_a$$

★ 当 \hat{A} 的本征值是两重简并。测量 \hat{A} 取值 a 时，并不知处于那一态，可能为

$$\alpha_1 u_a^{(1)} + \alpha_2 u_a^{(2)}$$

尽管 $\hat{B}u_a^{(1)}$ ， $\hat{B}u_a^{(2)}$ 都是 \hat{A} 的本征态。
但一般而言



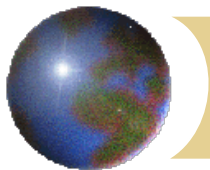
$$\hat{\mathbf{B}}\mathbf{u}_a^{(1)} = \mathbf{b}_{11}\mathbf{u}_a^{(1)} + \mathbf{b}_{21}\mathbf{u}_a^{(2)}$$

$$\hat{\mathbf{B}}\mathbf{u}_a^{(2)} = \mathbf{b}_{12}\mathbf{u}_a^{(1)} + \mathbf{b}_{22}\mathbf{u}_a^{(2)}$$

$$\hat{\mathbf{B}}\begin{pmatrix} \mathbf{u}_a^{(1)} \\ \mathbf{u}_a^{(2)} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_{11} & \mathbf{b}_{21} \\ \mathbf{b}_{12} & \mathbf{b}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_a^{(1)} \\ \mathbf{u}_a^{(2)} \end{pmatrix}$$

$$\hat{\mathbf{B}}\mathbf{v}_a^{(b_1)} = \mathbf{b}_1\mathbf{v}_a^{(b_1)}$$

$$\hat{\mathbf{B}}\mathbf{v}_a^{(b_2)} = \mathbf{b}_2\mathbf{v}_a^{(b_2)}$$



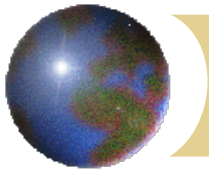
$$\mathbf{v}_a^{(b_i)} = \mathbf{c}_1^{(i)} \mathbf{u}_a^{(1)} + \mathbf{c}_2^{(i)} \mathbf{u}_a^{(2)}$$

代入

$$\hat{\mathbf{B}} \left(\mathbf{c}_1^{(i)} \mathbf{u}_a^{(1)} + \mathbf{c}_2^{(i)} \mathbf{u}_a^{(2)} \right) = \left(\mathbf{c}_1^{(i)}, \mathbf{c}_2^{(i)} \right) \hat{\mathbf{B}} \begin{pmatrix} \mathbf{u}_a^{(1)} \\ \mathbf{u}_a^{(2)} \end{pmatrix}$$

$$= \left(\mathbf{c}_1^{(i)}, \mathbf{c}_2^{(i)} \right) \begin{pmatrix} \mathbf{b}_{11} & \mathbf{b}_{21} \\ \mathbf{b}_{12} & \mathbf{b}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_a^{(1)} \\ \mathbf{u}_a^{(2)} \end{pmatrix}$$

$$= \left(\mathbf{b}_{11} \mathbf{c}_1^{(i)} + \mathbf{b}_{12} \mathbf{c}_2^{(i)}, \mathbf{b}_{21} \mathbf{c}_1^{(i)} + \mathbf{b}_{22} \mathbf{c}_2^{(i)} \right) \begin{pmatrix} \mathbf{u}_a^{(1)} \\ \mathbf{u}_a^{(2)} \end{pmatrix}$$

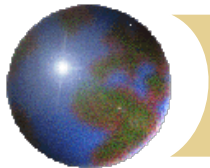


- $$= \mathbf{b}_i \left(\mathbf{c}_1^{(i)} \mathbf{u}_a^{(1)} + \mathbf{c}_2^{(i)} \mathbf{u}_a^{(2)} \right) = \mathbf{b}_i (\mathbf{c}_1^{(i)}, \mathbf{c}_2^{(i)}) \begin{pmatrix} \mathbf{u}_a^{(1)} \\ \mathbf{u}_a^{(2)} \end{pmatrix}$$

- $$(\mathbf{b}_{11} \mathbf{c}_1^{(i)} + \mathbf{b}_{12} \mathbf{c}_2^{(i)}, \mathbf{b}_{21} \mathbf{c}_1^{(i)} + \mathbf{b}_{22} \mathbf{c}_2^{(i)}) = \mathbf{b}_i (\mathbf{c}_1^{(i)}, \mathbf{c}_2^{(i)})$$

$$\begin{pmatrix} \mathbf{b}_{11} & \mathbf{b}_{12} \\ \mathbf{b}_{21} & \mathbf{b}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{c}_1^{(i)} \\ \mathbf{c}_2^{(i)} \end{pmatrix} = \mathbf{b}_i \begin{pmatrix} \mathbf{c}_1^{(i)} \\ \mathbf{c}_2^{(i)} \end{pmatrix}$$

$$\begin{vmatrix} \mathbf{b}_{11} - \mathbf{b} & \mathbf{b}_{12} \\ \mathbf{b}_{21} & \mathbf{b}_{22} - \mathbf{b} \end{vmatrix} = 0$$



可求得 $\hat{\mathbf{B}}$ 的本征值。若 $\mathbf{b}_1 \neq \mathbf{b}_2$ ，有

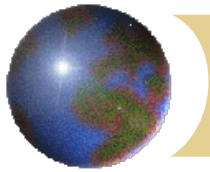
$$\mathbf{b}_{11}\mathbf{c}_1^{(1)} + \mathbf{b}_{12}\mathbf{c}_2^{(1)} = \mathbf{b}_1\mathbf{c}_1^{(1)}$$

$$\mathbf{b}_{21}\mathbf{c}_1^{(1)} + \mathbf{b}_{22}\mathbf{c}_2^{(1)} = \mathbf{b}_1\mathbf{c}_2^{(1)}$$

则

$$\mathbf{c}_2^{(1)} = \frac{(\mathbf{b}_1 - \mathbf{b}_{11})}{\mathbf{b}_{12}} \mathbf{c}_1^{(1)}$$

$$\mathbf{V}_a^{(\mathbf{b}_1)} = \mathbf{c}_1^{(1)} \left[\mathbf{u}_a^{(1)} + \frac{(\mathbf{b}_1 - \mathbf{b}_{11})}{\mathbf{b}_{12}} \mathbf{u}_a^{(2)} \right]$$

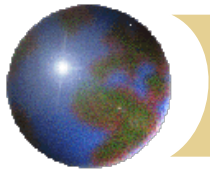


同理

$$\mathbf{V}_a^{(b_2)} = \mathbf{c}_1^{(1)} \left[\mathbf{u}_a^{(1)} + \frac{(\mathbf{b}_2 - \mathbf{b}_{11})}{\mathbf{b}_{12}} \mathbf{u}_a^{(2)} \right]$$

\hat{A}, \hat{B} 的本征值就唯一地决定波函数 $\mathbf{V}_a^{(b_i)}$ 。
它们的共同本征态没有一个是简并的。

力学量完全集：设力学量 $\hat{A}, \hat{B}, \hat{C} \dots$ 彼此对易；它们的共同本征函数 $u_{abc} \dots$ 是不简并的，也就是说，本征值 $a, b, c \dots$ 仅对应一个独立的本征函数，则称这一组力学量为力学量完全集。



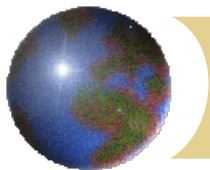
所以，以后要描述一个体系所处的态时，我们首先集中注意力去寻找一组独立的完全集，以给出特解，然后得到通解。

有了力学量完全集， $u_{nabc\dots}$ ，则可得

$$\psi(\underline{r}, t) = \sum_{n,a,b,c\dots} c_{nabc\dots} u_{nabc\dots} e^{-iE_n t / \hbar}$$

$$c_{nabc\dots} = \int u_{nabc\dots}^*(\underline{r}) \psi(\underline{r}, 0) d\underline{r}$$

\hat{L}^2, \hat{L}_z 完全集相应的本征函数组为 $Y_{lm}(\theta, \phi)$



V. 力学量平均值随时间的变化，运动常数，埃伦费斯脱定理 (Ehrenfest Theorem)

↑ A. 力学量的平均值随时间变化，运动常数

$$\bar{A} = (\psi(t), \hat{A}\psi(t))$$

它随时间演化为

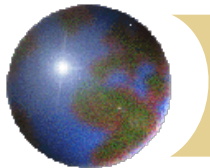


$$\frac{d\bar{A}}{dt} = \frac{d}{dt} \int \psi^*(\mathbf{r}, t) \hat{A} \psi(\mathbf{r}, t) d\mathbf{r}$$

$$= \int \frac{\partial \psi^*(\mathbf{r}, t)}{\partial t} \hat{A} \psi(\mathbf{r}, t) d\mathbf{r} + \int \psi^*(\mathbf{r}, t) \frac{\partial \hat{A}}{\partial t} \psi(\mathbf{r}, t) d\mathbf{r} + \int \psi^*(\mathbf{r}, t) \hat{A} \frac{\partial \psi(\mathbf{r}, t)}{\partial t} d\mathbf{r}$$

$$= \int \psi^*(\mathbf{r}, t) \frac{\partial \hat{A}}{\partial t} \psi(\mathbf{r}, t) d\mathbf{r} + \frac{1}{i\hbar} \int \psi^*(\mathbf{r}, t) \hat{A} \hat{H} \psi(\mathbf{r}, t) d\mathbf{r} - \frac{1}{i\hbar} \int (\hat{H} \psi(\mathbf{r}, t))^* \hat{A} \psi(\mathbf{r}, t) d\mathbf{r}$$

$$\frac{d\bar{A}}{dt} = \frac{\partial \hat{A}}{\partial t} + \frac{[\hat{A}, \hat{H}]}{i\hbar}$$

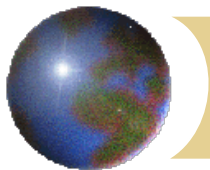


若 \hat{A} 不显含 t , 则

$$\frac{d\bar{A}}{dt} = \overline{[\hat{A}, \hat{H}]} \\ i\hbar$$

当 $[\hat{A}, \hat{H}] = 0$, 则 $\bar{\hat{A}}$ (对体系处于任何态) 不随 t 变, 而取 A_s 的概率 $\sum_n |c_{ns}|^2$ 也不随 t 变。

$$\frac{d\bar{A}}{dt} = 0$$

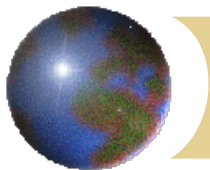


我们称与体系 \hat{H} 对易的不显含时间的力学量算符为体系的运动常数。

运动常数并不都能同时取确定值。因尽管它们都与 \hat{H} 对易，但它们之间可能不对易。如

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})$$

$\hat{L}^2, \hat{L}_x, \hat{L}_y, \hat{L}_z$ 都是运动常数，但 $\hat{L}_x, \hat{L}_y, \hat{L}_z$ 彼此不对易，不能同时取确定值。



B. 位力定理 (virial Theorem)

不显含 t 的力学量，在定态上的平均与 t 无关。

$$\frac{\overline{d\underline{r} \cdot \underline{\hat{p}}}}{dt} = \frac{\overline{[\underline{r} \cdot \underline{\hat{p}}, \hat{H}]}}{i\hbar} = 0,$$

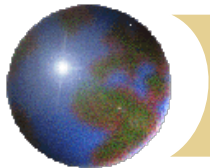
$$\frac{[\underline{r} \cdot \underline{\hat{p}}, \hat{H}]}{i\hbar} = \frac{1}{i\hbar} \left[\underline{r} \cdot \underline{\hat{p}}, \frac{\underline{\hat{p}}^2}{2m} \right] + \frac{1}{i\hbar} [\underline{r} \cdot \underline{\hat{p}}, V(\underline{r})]$$



$$\begin{aligned} &= \frac{1}{i\hbar} [\underline{\mathbf{r}}, \frac{\hat{\mathbf{p}}^2}{2m}] \cdot \hat{\mathbf{p}} + \frac{1}{i\hbar} \underline{\mathbf{r}} \cdot [\hat{\mathbf{p}}, V(\underline{\mathbf{r}})] \\ &= \frac{1}{i\hbar} \sum_i [x_i, \frac{\hat{\mathbf{p}}^2}{2m}] \cdot \hat{p}_i + \frac{1}{i\hbar} \sum_i x_i [\hat{p}_i, V(\underline{\mathbf{r}})] \\ &= \frac{\hat{\mathbf{p}}^2}{m} - \underline{\mathbf{r}} \cdot \nabla V(\underline{\mathbf{r}}) \end{aligned}$$

所以 $2\overline{\hat{T}} = \overline{\underline{\mathbf{r}} \cdot \nabla V(\underline{\mathbf{r}})}$

称为 virial Theorem 位力定理



若 $V(x, y, z)$ 是 x, y, z 的 n 次齐次函数，则

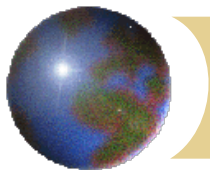
$$2\overline{\hat{T}} = n\overline{V(\underline{r})}$$

例：谐振子势是 x, y, z 的二次齐次函数

$$\overline{\hat{T}} = \overline{V(\underline{r})}$$

例：库仑势是 x, y, z 的 -1 次齐次函数

$$2\overline{\hat{T}} = -\overline{V(\underline{r})}$$



C. 能量-时间不确定关系

由算符间测量值的不确定关系，

$$\Delta\hat{A} \cdot \Delta\hat{B} \geq \frac{1}{2} \left| \overline{i[\hat{A}, \hat{B}]} \right|$$

取 $\hat{B} = \hat{H}$ ，则有

$$\Delta A \cdot \Delta E \geq \frac{1}{2} \left| \overline{i[\hat{A}, \hat{H}]} \right| = \frac{\hbar}{2} \left| \overline{\left[\hat{A}, \hat{H} \right]} \right|$$

若 \hat{A} 是不显含时间的算符，则有



$$\frac{d\bar{A}}{dt} = \frac{[\hat{A}, \hat{H}]}{i\hbar}$$

取

$$\tau_A = \frac{\Delta A}{\left| \frac{d\bar{A}}{dt} \right|}$$

则有

$$\tau_A \cdot \Delta E \geq \frac{\hbar}{2}$$

这即为能量和时间的不确定关系。