Quantum Mechanics

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量子力学的形式化

“如果人们不相信数学是简单的，那只是因为他们没有意识到生活是多么复杂。” ——约翰 冯 诺依曼

“科学建立在实验的基础上”，但“科学根植于对话。”——海森堡

“数学只是一种工具，我们应该学会把物理思想放在自己的头脑中，而不去参考数学的形式。”——保罗·狄拉克(Paul Dirac)

首先，我们体会一下前边一维模型定态薛定谔方程的求解思路和过程。我们通常从对体系的能量E和势能的大小比较分类开始，当设定粒子能量E低于势阱深度时，虽然我们不知道能量E的大小，但是认定粒子处于哈密顿量算符$\hat{H}$的本征态，及体系的能量就是本征方程$\hat{H}\psi = E\psi$中的本征值，而且该本征值在粒子可能出现的所有区域保持不变。然后，我们求解该本征方程，并在波函数的标准条件之下得到体系能量本征值和本征波函数。

这样的操纵告诉我们，如果量子力学体系处于某个用算符$\hat{F}$表示的力学量（不限于能量）的本征态时，这个力学量就有确定值，即，本征方程$\hat{F}\psi = \lambda\psi$中的本征值$\lambda$。这本质上上是量子力学的一个假设，其简单表述就是：“量子力学的力学量用算符表示”。

这样，就需要我们对力学量算符有一个全面深刻的描述。

再进一步思考，本征值和本征波函数有什么联系？对于同一个本征值的状态是不会随着本征波函数形式的改变而改变的，那么我们是否可以将波函数抽象为仅仅是一个状态，给予一个抽象的符号？

Chapter 3 Formalism

- 3.0 Linear Algebra
- 3.1 Hilbert space
- 3.2 Observables
- 3.3 Eigenfunctions of a Hermitian Opertor
- 3.4 The Generalized Statistical Interpretation
- 3.5 The Uncertainty Principle
- 3.6 Dirac Notation
- Summary

- **3.1 Hilbert space**

- Quantum theory is based on : **wave functions** and **operators**.
- The ***state*** of a system is represented by ***its wave function***, ***observable***s are represented by ***operator***s.
- Mathematically, wave functions satisfy the defining conditions for abstract vectors, and operators act on them as linear transformations.
- Apply the machinery of linear algebra to the case of **function spaces**, in which the ***"vectors" are (complex) functions of x, inner products are integrals, and derivatives appear as linear transformations***.

the inner product of functions $f(x)$, $g(x)$ is defined

$$\boxed{\langle f \mid g\rangle = \int_a^b f^*(x)g(x)dx}$$

$$\langle f \mid g\rangle = \langle g \mid f\rangle^*$$

$$\langle f \mid f\rangle \geq 0 \quad , \qquad \langle f \mid f\rangle = 0 \quad \Leftrightarrow \quad \mid f\rangle = 0$$

$$\langle f \mid ag\rangle = a\langle f \mid g\rangle$$

$$\langle af \mid g\rangle = a^*\langle f \mid g\rangle \qquad , \quad \text{a is scalar}$$

$$\langle f \mid (a \mid g\rangle + b \mid h\rangle\,) = a\langle f \mid g\rangle + b\langle f \mid h\rangle$$

the inner product must ***converge*** , every admissible function f must be **square integrable**

$$\int |f(x)|^2 \, dx < \infty$$

the set of all **square integrable functions,** on a specified interval

$$f(x) \quad \text{such that} \quad \int_a^b |\mathrm{f(x)}|^2 \, dx < \infty,$$

constitutes a vector space, called **Hibert space**.

Normalized function: its inner product with itself is 1.

Two functions are **orthogonal** if their inner product is 0.

$$\langle f_m | f_n \rangle = \delta_{mn}$$

A set of functions is **complete** if any other function (in Hibert space) can be expressed as a linear combination of them

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

$$c_n = < f_n(x) | f(x) >$$

For example, consider the set $P(N)$ of all *polynomials* of degree $< N$:

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{N-1} x^{N-1},$$

on the interval $-1 \leq x \leq 1$. They are certainly square integrable, so this is a bona fide inner product space. An obvious basis is the set of powers of x:

$$|e_1\rangle = 1,\ |e_2\rangle = x,\ |e_3\rangle = x^2,\ \ldots,\ |e_N\rangle = x^{N-1};$$

evidently it's an N-dimensinal vector space. This is *not*, however, an *orthonormal* basis, for

$$\langle e_1|e_1\rangle = \int_{-1}^{1} 1\, dx = 2, \quad \langle e_1|e_3\rangle = \int_{-1}^{1} x^2\, dx = 2/3,$$

and so on. If you orthonormalize this basis, you get the famous Legendre polynomials

$$|e'_n\rangle = \sqrt{n-(1/2)}\,P_{n-1}(x), \quad (n = 1, 2, \ldots, N).$$

$$P_0 = 1$$
$$P_1 = x$$
$$P_2 = \tfrac{1}{2}(3x^2 - 1)$$
$$P_3 = \tfrac{1}{2}(5x^3 - 3x)$$
$$P_4 = \tfrac{1}{8}(35x^4 - 30x^2 + 3)$$
$$P_5 = \tfrac{1}{8}(63x^5 - 70x^3 + 15x)$$

- **3.2 Observables**
- 算符

算符

算符：指作用在一个函数上得出另一个函数的运算符号。

比如：$\frac{\partial}{\partial x}$，$\sqrt{\ }$

算符本身没有任何具体物理内容，只有把它作用在状态是，才体现其含义。

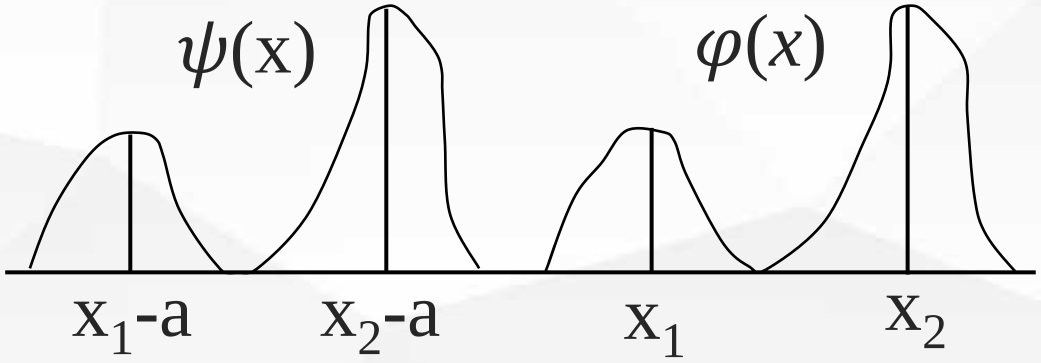
算符

设某种运算$\hat{F}$ 把函数$\psi(x,y,z,t)$变为$\varphi(x,y,z,t)$，用符号表示为

$$\hat{F}\psi = \varphi$$

量子力学中这运算代表一个变换，使空间分布的几率振幅

$$\psi(x,y,z,t) \xrightarrow{\hat{F}} \varphi(x,y,z,t)$$



例如 $\hat{F} = \mathrm{e}^{-iap_x/\hbar}$的作用

量子力学对算符的要求

量子力学中常见的算符

动量算符

哈密顿量算符

$$\hat{p} = -i\hbar\nabla, \hat{H} = i\hbar\frac{\partial}{\partial t}$$

$$\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + V(\boldsymbol{r})$$

量子力学对算符的要求

量子力学基本假设

力学量由相应的算符表示。即每个力学量A存在一个相应的力学量算符$\hat{A}$，它在由波函数所表示的状态中的平均值为

$$\langle \mathrm{A} \rangle = \int \Psi^{*} \hat{A} \Psi dV$$

量子力学中态叠加原理和力学量测量值是实数的要求，则算符必须是线性+厄密算符

线性算符及性质

满足$\hat{A}(c_1\psi_1 + c_2\psi_2) = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$的算符——线性算符

例 $\frac{\partial}{\partial x}$是线性算符，$\sqrt{\ }$不是。

- 单位算符$\hat{I}$是保持波函数不改变的算符
- 线性算符之和 $(\hat{A} + \hat{B})\Psi = \hat{A}\Psi + \hat{B}\Psi$
- 线性算符之积$(\hat{A}\hat{B})\Psi = \hat{A}(\hat{B}\Psi)$一般说算符之积不满足交换律，$\hat{A}\hat{B} \neq \hat{B}\hat{A}$

算符的幂 $\hat{A}^n\hat{A}^m = \hat{A}^{n+m}$

线性算符性质（续）

- 加法交换律 $\hat{A}+\hat{B}=\hat{B}+\hat{A}$
- 加法结合律 $\hat{A}+\hat{B}+\hat{C}=\hat{A}+(\hat{B}+\hat{C})=(\hat{A}+\hat{B})+\hat{C}$
- 乘法分配律 $\hat{C}(\hat{A}+\hat{B})=\hat{C}\hat{A}+\hat{C}\hat{B}$
- 乘法结合律 $\hat{A}\hat{B}\hat{C}=\hat{A}(\hat{B}\hat{C})=(\hat{A}\hat{B})\hat{C}$

线性算符及性质

- 逆算符：设从$\hat{F}\psi = \varphi$能唯一解出ψ，则定义的逆算符 $\hat{F}^{-1}\varphi = \psi$

注意:不是所有的逆算符都有逆算符

- 逆算符满足 $\hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I}$, $\left(\hat{A}\hat{B}\right)^{-1} = \hat{B}^{-1}\hat{A}^{-1}$

算符高级运算

算符的复共轭，

两个任意波函数Ψ和φ的标量积定义： $(\Psi,\varphi)=\int dV\Psi^*\varphi$ ，具有如下性质

$$(\Psi,\Psi)\geq 0,\qquad (\Psi,\varphi)^*=(\varphi,\Psi)$$

$$(\Psi,c_1\varphi_1+c_2\varphi_2)=c_1(\Psi,\varphi_1)+c_2(\Psi,\varphi_2)$$

$\hat{Q}$中所有复量换成其共轭复量就得到其复共轭算符$\hat{Q}^*$

$$\left(\hat{A}\hat{B}\hat{C}\right)^*=\hat{A}^*\hat{B}^*\hat{C}^*$$

算符高级运算

算符的转置

$\hat{Q}$转置算符$\tilde{\hat{Q}}$定义为满足$\left(\Psi,\tilde{\hat{Q}}\varphi\right) = (\varphi^*,\hat{Q}\Psi^*)$,即

$$\int dV\Psi^*\tilde{\hat{Q}}\varphi = \int dV\varphi\hat{Q}\Psi^*$$

- 满足 $$\widetilde{\hat{A}\hat{B}} = \tilde{\hat{B}}\tilde{\hat{A}}$$

厄密算符

$\hat{Q}$的厄密共轭算符：　$\hat{Q}^{+}=\tilde{\hat{Q}}^{*}$——转置复共轭

- 所以　$(\Psi,\hat{Q}^{+}\varphi)=(\hat{Q}\Psi,\varphi),(\hat{A}\hat{B})^{+}=\hat{B}^{+}\hat{A}^{+}$

厄密算符

厄密算符（自共轭算符）是满足下列关系的算符

$$\boxed{\hat{Q}^{+}=\hat{Q}}$$

- 所以　$\int dV\Psi^{*}\hat{Q}\varphi=\int dV(\hat{Q}\Psi)^{*}\varphi$
- 如果　$\boxed{\hat{Q}^{+}=-\hat{Q}\text{——反厄密算符}}$

厄密算符性质

1. 厄密算符相加、减仍是厄密算符；但厄密算符之积（$(\hat{A}\hat{B}\hat{C})^{+}=\hat{C}^{+}\hat{B}^{+}\hat{A}^{+}$）并不一定为厄密算符.

2. 任何状态下，厄密算符的平均值必为实数.

3. 两个厄密算符的乘积一定可以表示为一个厄密算符和一份反厄密算符的和。

厄密算符性质

证明 $$\hat{A}\hat{B}=\frac{1}{2}(\hat{A}\hat{B}+\hat{B}\hat{A})+\frac{1}{2}(\hat{A}\hat{B}-\hat{B}\hat{A})$$

设 $\hat{F}=\frac{1}{2}(\hat{A}\hat{B}+\hat{B}\hat{A})$, $\hat{G}=\frac{1}{2}(\hat{A}\hat{B}-\hat{B}\hat{A})$, 则

$$\hat{F}^{+}=\hat{F}\ ,\ \hat{G}^{+}=-\hat{G}$$

如$\hat{A}\hat{B}-\hat{B}\hat{A}=0$，则乘积是厄密算符

Example 1. momentum operator $\hat{p}$ is Hermitian

$$\langle\Psi|\hat{p}\Psi\rangle=\int\Psi^*(-i\hbar\frac{d}{dx})\Psi dx=-i\hbar\left[\left(\Psi^*\Psi\right)_{-\infty}^{\infty}-\int\Psi\frac{d}{dx}\Psi^*dx\right]$$

$$=\int\Psi(-i\hbar\frac{d}{dx}\Psi)^*dx=\langle\hat{p}\Psi|\Psi\rangle$$

2. Hamiltonian operator $\hat{H}$ is Hermitian

$$\langle \Psi \mid \hat{H}\Psi \rangle = \langle \Psi \mid (-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V)\Psi \rangle = \langle \Psi \mid (-\frac{\hbar^2}{2m}\frac{d^2}{dx^2})\Psi \rangle + V\langle \Psi \mid \Psi \rangle$$

$$= -\frac{\hbar^2}{2m}\int \Psi^* \frac{d^2}{dx^2}\Psi dx + V\int |\Psi|^2 dx$$

$$= -\frac{\hbar^2}{2m}\left[\left(\Psi^* \frac{d\Psi}{dx}\right)_{-\infty}^{\infty} - \int \frac{d\Psi}{dx}\frac{d\Psi^*}{dx}dx\right] + V\int |\Psi|^2 dx$$

$$= \frac{\hbar^2}{2m}\left[\left(\Psi \frac{d\Psi^*}{dx}\right)_{-\infty}^{\infty} - \int \Psi \frac{d^2\Psi^*}{dx^2}dx\right] + V\int |\Psi|^2 dx$$

$$= \int \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)\Psi^*\Psi dx = \int \hat{H}\Psi^*\Psi dx$$

$$= \int (\hat{H}\Psi)^*\Psi dx = \langle \hat{H}\Psi \mid \Psi \rangle$$

作业（提示计算$(\Psi, \hat{Q}^+\varphi)$）

- 1. 计算常数算符的共轭算符
- 2. 求算符$\partial/\partial x$ 的共轭算符
- 3.求算符$i\partial/\partial x$ 的共轭算符
- 4. 证明算符$i\partial/\partial x$ 是厄密算符
- 5. 计算$\hat{L}_z = x\hat{p}_y - y\hat{p}_x$的共轭算符,判断是否厄密算符

- **3.3 Eigenfunctions of a Hermitian Opertor**
- 线性厄密算符的本征函数

力学量算符假定

量子力学基本假定

每一个经典力学量在量子力学中都对应一个线性厄密算符，测量力学量O时，所有可能出现的值，都是力学量算符$\hat{O}$的本征值。

原因1 厄密算符的本征值必为实数

证 设 $\hat{F}\psi=\lambda\psi$

$\hat{F}$为厄密算符 $\int dV\Psi^*\hat{Q}\varphi=\int dV(\hat{Q}\Psi)^*\varphi$

取 $\varphi=\Psi$，$\lambda\int dV\Psi^*\Psi=\lambda^*\int dV\Psi^*\Psi$ 得到 $\lambda=\lambda^*$ ，所以λ是实数

力学量算符假定

原因2 态叠加原理决定了力学量算符必须为线性算符

证 设 $\hat{H}\psi_1 = E\psi_1, \hat{H}\psi_2 = E\psi_2$

因为 $\psi = c_1\psi_1 + c_2\psi_2$

也应是体系的态，有 $\hat{H}\psi = E\psi$

则 $\hat{H}(c_1\psi_1 + c_2\psi_2) = E(c_1\psi_1 + c_2\psi_2) = c_1\hat{H}\psi_1 + c_2\hat{H}\psi_2$

所以$\hat{H}$为线性算符

力学量算符的本征值和本征函数

设体系处于Ψ

测量力学量O，一般来说，可能出现不同结果，各有一定的几率，多次测量结果的平均值趋于一确定值，每次具体测量的结果围绕平均值有一个涨落

$$\overline{\Delta O^2} = \overline{(\hat{O} - \overline{O})^2} = \int \Psi^* (\hat{O} - \overline{O})^2 \Psi dV$$

如$\hat{O}$为厄密算符，$\hat{O} - \overline{O}$也是厄密算符

$$\int \Psi^* (\hat{O} - \overline{O})^2 \Psi dV = \int [(\hat{O} - \overline{O})\Psi]^* (\hat{O} - \overline{O})\Psi dV = \int |(\hat{O} - \overline{O})\Psi|^2 dV \geq 0$$

力学量算符的本征值和本征函数

存在特殊状态

The standard deviation of Q, in determinate state, is zero.

测量力学量O所得结果完全确定。即$\overline{\Delta O^2} = 0$——力学量$O$的本征态。

在这种状态下

determinate states

The average is O_n, and every measurement gives O_n， so

$$(\hat{O} - \overline{O})\Psi = 0 \Longrightarrow \hat{O}\Psi_n = O_n\Psi_n$$

is the eigenvalue equation for the operator $\hat{O}$, $\Psi_n$is an eigenfunction of it and O_n is the corresponding eigenvalue, thus

Determinate states are eigenfunctions of $\hat{O}$.

算符的本征值和本征函数

- 如果算符$\hat{F}$作用于一个函数ψ，结果等于ψ乘上一个常数 λ

$$\hat{F}\psi = \lambda\psi$$

- 则称λ为$\hat{F}$的本征值，ψ为属于λ的本征函数，上式称为算符$\hat{F}$的本征值方程。

- 显然定态薛定谔方程 $\hat{\mathrm{H}}\psi = \lambda\psi$ 就是哈密顿量算符的本征方程

For every observable quantity, A, there is an associated Hermitian operator, **A**, such that:

$$\mathbf{A}\psi = \lambda\psi$$

In fact, if there are *n* allowed states then there are *n* eigenfunctions, ψ_i, that satisfy:

$$\mathbf{A}\psi_i = \lambda_i\psi_i$$

The result of making a measurement of A is one of the eigenvalues of A. That is, only a limited set of outcomes are possible (discrete nature of quantum mechanics).

What is the value we might expect to measure? **Expectation Value**

The expectation value is the average magnitude of a property sampled over an ensemble of identically prepared systems. The expectation value, <A>, is the scalar product of Ψ and $\mathbf{A}\Psi$:

$$\langle A \rangle = \int \Psi^* \mathbf{A} \Psi d\tau$$

If the wavefunction is an eigenfunction of the operator ($\Psi = \psi_n$):

$$\langle A \rangle = \int \Psi^* \mathbf{A} \Psi d\tau = \int \psi_n^* \mathbf{A} \psi_n d\tau = \lambda_n \int \psi_n^* \psi_n d\tau = \lambda_n$$

In general $\Psi \neq \psi_n$, but

$$\Psi = \sum_{i=1}^{N} c_i \psi_i$$

$$\langle \mathbf{A} \rangle = \int \Psi * \mathbf{A} \Psi \, d\tau$$

$$= \int \left[\sum_{i=1}^{N} c_i \psi_i \right] * \mathbf{A} \left[\sum_{j=1}^{N} c_j \psi_j \right] d\tau \qquad = \int \left[\sum_{i=1}^{N} c_i^* \psi_i^* \right] \mathbf{A} \left[\sum_{j=1}^{N} c_j \psi_j \right] d\tau$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} c_i^* c_j \int \psi_i^* \mathbf{A} \psi_j \, d\tau \qquad noting: \quad A\psi_j = \lambda_j \psi_j$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} c_i^* c_j \lambda_j \int \psi_i^* \psi_j \, d\tau \qquad noting: \quad \int \psi_i^* \psi_j \, d\tau = \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

$$= \sum_{j=1}^{N} c_j^* c_j \lambda_j = \sum_{j=1}^{N} c_j^2 \lambda_j$$

probability that c_j is obtained in a single measurement

What does this mean?

When A is measured for a single member of an ensemble, the result is one of the eigenvalues of A, but which one cannot be predicted in advance.

The result means that the eigenvalue λ_j will be obtained in a single measurement with the probability of c_j^2.

So, **for a single measurement, there are specified values of A that are possible, but over an ensemble, the expectation value <A> can be a continuous value.**

The collection of all the eigenvalues of an operator is called its **spectrum**, If two (or more) linearly independent eigenfunctions share the same eigenvalue, the spectrum is said to be **degenerate**.

Example Consider the operator $\hat{Q} \equiv i\frac{d}{d\phi}$, where ϕ is the usual polar coordinate in two dimensions. Is $\hat{Q}$ hermitian? Find its eigenfunctions and eigenvalues.

Solution: Here we are working with functions $f(\phi)$ on the finite interval $0 \le \phi \le 2\pi$, and stipulate (约定) that

$$f(\phi + 2\pi) = f(\phi)$$

Since ϕ and $\phi+2\pi$ describe the same physical point. Using integration by parts

$$\left\langle f \middle| \hat{Q} g \right\rangle = \int_0^{2\pi} f^* \left(i \frac{dg}{d\phi} \right) d\phi = i f^* g \Big|_0^{2\pi} - \int_0^{2\pi} i \frac{df^*}{d\phi} g \, d\phi = \left\langle \hat{Q} f \middle| g \right\rangle$$

So Q is hermitian.

The eigenvalue equation, $i \frac{df(\phi)}{d\phi} = q f(\phi)$,

has the general solution $f(\phi) = A e^{-iq\phi}$.

The periodic condition restricts the possible values of the q

$$e^{-iq2\pi} = 1 \Rightarrow q = 0, \pm 1, \pm 2, \cdots$$

The spectrum is the set of all integers, and it is nondegenerate.

算符的本征值和本征函数

理解：

如果知道算符的具体形式，根据一定的边界条件，即可解出其本征函数和本征值。本征值可能是连续的，也可能是分立的。 本征值的集合称为**本征值谱**。 所有本征函数的集合称为**本征基**。

Matrix Representation of Operators

Solving the Schrödinger equation (DIFFERENTIAL form) will be more convenient to utilize a MATRIX form

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r})$$

To develop this matrix form, we begin by rewriting the SE as

$$H\psi = E\psi \qquad (S.1)$$

Next we note that the wavefunction can be written as a linear SUPERPOSITION of the eigenfunctions of some arbitrary operator

$$\psi = \sum_n a_n \varphi_n \qquad (S.2)$$

Next we introduce Eq. S.2 into Eq. S.1 so that the SE becomes

$$H\sum_n a_n\varphi_n = E\sum_n a_n\varphi_n \quad \Rightarrow \quad \sum_n a_n H\varphi_n = E\sum_n a_n\varphi_n \qquad (S.3)$$

Next we multiply from the left by $\varphi_m{}^*$ and integrate to obtain

$$\sum_n a_n\int\varphi_m^* H\varphi_n = E\sum_n a_n\int\varphi_m^*\varphi_n \qquad (S.4)$$

The integral on the RHS of Eq. S.4 is just the orthonormality condition for the eigenfunctions and immediately reduces to δ_{mn}

To simplify the form of the LHS of Eq. S.4 we define the so-called MATRIX ELEMENT H_{mn}

$$H_{mn} = \int\varphi_m^* H\varphi_n \equiv \langle m|H|n\rangle \qquad (S.5)$$

• Then SE can be rewritten as

$$\sum_n H_{mn} a_n = E\, a_m \qquad (S.6)$$

* This is now an eigenvalue equation in which the Hamiltonian is expressed in MATRIX form

$$\mathrm{H}\mathbf{a} = E\mathbf{a} \qquad (S.7)$$

$$\mathrm{H} = \begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1n} \\ H_{21} & H_{22} & \cdots & H_{2n} \\ \vdots & \vdots & & \vdots \\ H_{n1} & H_{n2} & \cdots & H_{nn} \end{bmatrix} \qquad (S.8) \qquad \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \qquad (S.9)$$

$\Rightarrow$ Note that the DIMENSION of the matrix form of H is determined by the number of unique eigenfunctions and can often be INFINITE!

• To determine the energy eigenvalues from Eq. S.7 we rewrite it as

$$(\mathrm{H}-E)\mathbf{a}=\mathbf{0} \qquad (S.10)$$

$$\det|\mathrm{H}-E|=\mathbf{0} \qquad (S.11)$$

* The condition for this equation to have nontrivial solutions is that its determinant should VANISH

$$\begin{vmatrix} H_{11}-E & H_{12} & H_{13} & \dots & H_{1n} \\ H_{21} & H_{22}-E & H_{23} & \dots & H_{2n} \\ & & \vdots & & \\ & & \vdots & & \\ H_{n1} & H_{n2} & H_{n3} & \dots & H_{nn}-E \end{vmatrix}=0 \qquad (S.12)$$

* For an $n \times n$ matrix solution of this determinant yields n INDEPENDENT simultaneous equations and thus n independent solutions for the energy.

- We know that the operators must be HERMITIAN to ensure that their eigenvalues are real
  The corresponding matrix representation of any operator must similarly ALSO be Hermitian
  A Hermitian matrix may be DEFINED as one whose elements are related according to

$$M_{mn} = M^*_{nm} \quad \Rightarrow \quad \mathrm{M} = \begin{bmatrix} M_{11} & M_{12} & \dots & M_{1n} \\ M^*_{12} & M_{22} & \dots & M_{2n} \\ \vdots & \vdots & & \vdots \\ M^*_{1n} & M^*_{2n} & \dots & M_{nn} \end{bmatrix} \qquad (S.13)$$

The notation $< m \,|\, H \,|\, n >$ for the matrix elements is due to DIRAC and $< m \,|$ is referred to as the BRA while $|\, n >$ is referred to as the KET

* Note that the Dirac form keeps only the indices n and m that label the eigenfunctions φ

- While we have expressed the Hamiltonian in terms of matrix elements involving the eigenfunctions φ_n of an ARBITRARY operator it is natural to use the eigenfunctions of the Hamiltonian itself so that the matrix elements become

$$H_{mn} = \int \varphi_m^* H \varphi_n = \int \varphi_m^* E_n \varphi_n = E_n \delta_{mn} \qquad (S.14)$$

* This matrix is DIAGONAL since all off-diagonal elements are equal to ZERO

* It is possible that OTHER operators may also be diagonal when expressed using the Eigenfunctions that diagonalize the Hamiltonian

$$[Q, H] = 0 \qquad (S.15)$$

$\Rightarrow$ This can only happen if the two operators **COMMUTE.**

1 Discrete spectra

The normalizable eigenfunctions of a hermitian operator have two important properties.

Theorem 1: The eigenvalues of a hermitian operator are real.

Theorem 2: eigenfunctions belonging to distinct eigenvalues are orthogonal.

Axiom: *The eigenfunctions of an observable operator are complete: any function can be expressed as a linear combination of them.*

For the **degenerate eigenvalue**, if two (or more) eigenfunctions share the same eigenvalue, we can use the **Gram-Schmidt orthogonalization procedure** to construct orthogonal eigenfunctions within each degenerate subspace.

2 Continuous spectra

If the spectrum of a hermitian operator is continuous, the eigenfunctions are *not normalizable*. Nevertheless, there is a sense in which the three essential properties (reality, orthogonal, and completeness) still hold.

Example: Find the eigenfunctions and eigenvalues of the momentum operator.

Solution: Let $f_p(x)$ be the eigenfunction and p the eigenvalue:

$$\frac{\hbar}{i}\frac{d}{dx}f_p(x)=pf_p(x)\Rightarrow f_p(x)=Ae^{ipx/\hbar}$$

This is not square-integrable, for any value of p, ----the momentum operator has no eigenfunctions in Hilbert space, but

$$\int_{-\infty}^{+\infty} f_{p'}^{*}(x)f_p(x)dx=|A|^2\int_{-\infty}^{+\infty} e^{i(p-p')x/\hbar}=|A|^2 2\pi\hbar\delta(p-p')$$

If we pick $A=1/\sqrt{2\pi\hbar}$, so that

$$f_p(x)=\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar},\Rightarrow\langle f_{p'}|f_p\rangle=\delta(p-p')$$ **Dirac orthonormality.**

Example Find the eigenfunctions and eigenvalues of the position operator.

Solution: Let $g_y(x)$ be the eigenfunction and y the eigenvalue:

$$xg_y(x) = yg_y(x) \Rightarrow g_y(x) = A\delta(x-y)$$

This is not square-integrable, for any value of y, but again they admit dirac orthonormality:

$$\int_{-\infty}^{+\infty} g_{y'}^*(x) g_y(x) dx = |A|^2 \int_{-\infty}^{+\infty} \delta(x-y')\delta(x-y) dx = |A|^2 \delta(y-y')$$

If we pick A=1, so

$$g_y(x) = \delta(x-y) \Rightarrow \langle g_{y'} | g_y \rangle = \delta(y-y')$$

Construction of an Hermitian operator

To translate the classical quantity xp_x into a quantum mechanical operator.

Solution: Since the operators $x\ and\ p_x$ do not commute

$$p_x x - x p_x = \frac{\hbar}{i}$$

It is easily checked in the Schrodinger equation representation $p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$,

we expect every operator

$$\Omega = (1-\alpha)xp_x + \alpha p_x x$$

to correspond to the classical quantity xp_x. Let us first suppose the constantα to be real.

Construction of an Hermitian operator

It must now be determined in such a way that the expectation value of Ω in any quantum state described by a wave function ψ is a real number, so we get

$$\langle\Omega\rangle = \frac{\hbar}{i}\int d^3x\psi^*\{(1-\alpha)x\frac{\partial\psi}{\partial x} + \alpha\frac{\partial(x\psi)}{\partial x}\} = \frac{\hbar}{i}\int d^3x\psi^*\{x\frac{\partial\psi}{\partial x} + \alpha\psi\}$$

Breaking up $\psi = f + ig$ into its real and imaginary parts, this leads to

$$\langle\Omega\rangle = \frac{\hbar}{i}\int d^3x\left\{x\left(f\frac{\partial f}{\partial x} + g\frac{\partial g}{\partial x}\right) + \alpha(f^2 + g^2)\right\} + \hbar\int d^3x\, x\left(f\frac{\partial g}{\partial x} - g\frac{\partial f}{\partial x}\right)$$

The first term being purely imaginary must vanish.

Construction of an Hermitian operator

Since $$\int d^3x\ (f^2+g^2)=1$$

this condition may be written

$$\int d^3x\, x\left(f\frac{\partial f}{\partial x}+g\frac{\partial g}{\partial x}\right)=-\alpha,\ \text{or}\ \frac{1}{2}\int d^3x\, x\frac{\partial}{\partial x}(f^2+g^2)=-\alpha,$$

by partial integration $\alpha=\frac{1}{2}$. So that the symmetrical combination

$$\Omega=\frac{1}{2}(xp_x+p_x x)$$

is the correct, because Hermitian, operator.

Construction of an Hermitian operator

If we admit complex values of α, any value $\alpha = \frac{1}{2} + i\beta$ with arbitrary real β will do, because it leads to

$$\Omega = \frac{1}{2}(xp_x + p_x x) + i\beta(p_x x - xp_x)$$

the first part to have a real expectation value,

the second part will in consequence of the commutation relation become the real constant $\beta\hbar$, independent of the special quantum state. **This term therefore has no physical significance and may be omitted.**

厄密算符本征函数性质力学量算符平均值

厄密算符本征函数正交性

1.正交性

- 厄密算符属于不同本征值的本征函数彼此正交。
- 如果两函数ψ_1和ψ_2满足$\int \psi_1^* \psi_2 dV = 0$，积分是对变量变化的全部区域进行,则称$\psi_1$和$\psi_2$相互正交。

证 设 $\hat{F}\psi_1 = \lambda_1 \psi_1$， $\hat{F}\psi_2 = \lambda_2 \psi_2$， $\lambda_1 \neq \lambda_2$

则 $\left(\hat{F}\psi_1\right)^* = \lambda_1 \psi_1^*$

$$\int \left(\hat{F}\psi_1\right)^* \psi_2 dV = \lambda_1 \int \psi_1^* \psi_2 dV$$

$$\int \psi_1^* (\hat{F}\psi_2) dV = \lambda_2 \int \psi_1^* \psi_2 dV$$

厄密算符本征函数正交性

- 厄密算符性质$\int (\hat{F}\psi_1)^* \psi_2 dV = \int \psi_1^* (\hat{F}\psi_2) dV$

则 $\lambda_1 \int \psi_1^* \psi_2 dV = \lambda_2 \int \psi_1^* \psi_2 dV$,

因为$\lambda_1 \neq \lambda_2$，只能 $\int \psi_1^* \psi_2 dV = 0$

这里只考虑分离谱,对连续谱也是成立的对归一化的本征函数

$$\int \psi_k^* \psi_l dV = \delta_{kl}$$

分离谱

$$\int \psi_\lambda^* \psi_{\lambda'} dV = \delta(\lambda - \lambda')$$

连续谱

这样的本征函数构成正交归一系

厄密算符简并本征函数的处理

- 当算符$\hat{F}$的多个本征函数对应同一个本征值，称为简并情况

$$\hat{F}\psi_{ni} = \lambda_n \psi_{ni}\ (i = 1,2,\cdots d)$$

- 如这些本征函数不一定正交。设

$$\int \psi_{\mathrm{ni}}^{*} \psi_{nj} dV = S_{ij}$$

- 用d个本征函数组合d个新函数

$$\varphi_{n\alpha} = \sum_{i} c_{\alpha i}\, \psi_{ni}, (\alpha = 1,2,\cdots d)$$

厄密算符简并本征函数的处理

- $\varphi_{n\alpha}$也是算符$\hat{F}$的本征函数

$$\hat{F}\varphi_{n\alpha} = \sum_i c_{\alpha i}\, \hat{F}\psi_{ni} = \lambda_n \sum_i c_{\alpha i}\, \psi_{ni} = \lambda_n \varphi_{n\alpha},$$

而

$$\int \varphi_{\mathrm{n}\alpha}^{*}\varphi_{n\beta}dV = \sum_{i=1}^{d}\sum_{j=1}^{d} c_{\alpha i}^{*}c_{\beta j}\int\int \psi_{\mathrm{n}i}^{*}\psi_{nj}dV = \sum_{i=1}^{d}\sum_{j=1}^{d} c_{\alpha i}^{*}c_{\beta j}\, S_{ij}$$

厄密算符简并本征函数的处理

- 选择$c_{\alpha i}$使得 $$\sum_{i=1}^{d}\sum_{j=1}^{d} c_{\alpha i}^{*} c_{\beta j} S_{ij} = \delta_{\alpha\beta}$$

  重新组合d个正交函数。

- 选择$c_{\alpha i}$的方式有多种，比如对2度简并：$\hat{F}\psi_{n1} = \lambda_n \psi_{n1}$，$\hat{F}\psi_{n2} = \lambda_n \psi_{n2}$，可以让一个本征函数为 $\varphi_{n1} = \psi_{n1}$，另一个为 $\varphi_{n2} = a_1\psi_{n1} + a_2\psi_{n2}$, 选择

$$\boxed{\frac{a_1}{a_2} = -\frac{\int \psi_{\mathrm{n}1}^{*}\psi_{n2}\,dV}{\int \psi_{\mathrm{n}1}^{*}\psi_{n1}\,dV}}$$

  则φ_{n1}，φ_{n2}正交。

厄密算符本征函数系的完备性

2. 完备性

- 只要任意波函数$\Psi(x)$与本征波函数$\psi_n(x)$具有相同的边界条件，$\Psi(x)$可展开成所有本征函数$\psi_n(x)$的线性叠加

$$\Psi(x) = \sum_n c_n \psi_n(x)$$

本征函数的这种性质称为完备性，物理意义就是态叠加原理。

厄密算符本征函数系的完备性

$$\langle F\rangle = \int \Psi^* \hat{F}\Psi dV = \sum_{m,n} c_m^* c_n \int \psi_m^* \hat{\mathrm{F}}\psi_n dV = \sum_{m,n} c_m^* c_n \lambda_n \delta_{mn} = \sum_n |c_n|^2 \lambda_n$$

粒子处于力学量算符$\hat{F}$本征态时ψ_n，测量该力学量有一确定值λ_n。而在任意态Ψ时，测量该力学量无确定值！只有可能值$\lambda_1, \lambda_2, \cdots$，其出现几率为$|c_n|^2$，该力学量的期待值（平均值）由上式给出。

厄密算符本征函数系的完备性

- 如$\Psi(x)$是归一化的

$$1=\int \Psi^*\Psi dV=\sum_{m,n} c_m^* c_n \int \psi_m^*\psi_n dV=\sum_{m,n} c_m^* c_n\,\delta_{mn}=\sum_n |c_n|^2=1$$

- c_n与x无关,利用ψ_n的正交归一性，将ψ_m^*等式两边，对x在整个区域积分

$$\int \psi_m^*\Psi dV=\sum_n c_n\int \psi_m^*\psi_n dV=\sum_n c_n\,\delta_{mn}=c_m,$$

$$c_n=\int \psi_n^*\Psi dV$$

厄密算符本征函数系的完备性

- 对连续谱, $\hat{F}\psi_k = \lambda_k\psi_k$; 任意态展开:$\Psi(x) = \int c_k\psi_k(x)dk$,

  同样 $c_k = \int \psi_k^*\Psi dV$

- 当归一化 $\Psi(x) = \sum_n c_n\psi_n(x) + \int c_k\psi_k(x)dk$

$$\boxed{\langle F\rangle = \int \Psi^*\hat{F}\Psi dV = \sum_n |c_n|^2\lambda_n + \int |c_k|^2\lambda_k dk}$$

厄密算符本征函数系的封闭性

3. 封闭性

任意波函数$\Psi(x)$

$$\Psi(x)=\sum_n c_n\psi_n(x),\quad c_n=\int\psi_n^*\Psi dx$$

把c_n带入$\Psi(x)$

$$\Psi(x)=\sum_n c_n\psi_n(x)=\sum_n\int\psi_n^*(x')\Psi(x')dx'\,\psi_n(x)$$

$$=\int\Psi(x')\left[\sum_n\psi_n^*(x')\psi_n(x)\right]dx'$$

厄密算符本征函数系的封闭性

显然有

$$\sum_n \psi_n^*(x')\psi_n(x) = \delta(x-x') \Rightarrow$$

本征函数的封闭性。

连续谱时封闭性条件为

$$\int \psi_k^*(x')\psi_k(x)dk = \delta(x-x')$$

同时存在分立和连续谱

$$\sum_n \psi_n^*(x')\psi_n(x) + \int \psi_k^*(x')\psi_k(x)dk = \delta(x-x')$$

厄密算符本征函数的性质

量子力学中的算符，除满足线性厄密外，还要其全部本征函数能够组成完备系，满足这些条件的算符称为观测量。所有正交归一化的一套本征函数系是构成状态描述的基石。

讨论:

(1) 当$\Psi(x)$是算符$\hat{F}$的一个本征函数时,$\Psi(x)=\psi_n$,即$c_n=1$,其它系数为零，这时测量力学量的测量值必是λ_n

(2) 当$\Psi(x)$不是算符$\hat{F}$的本征函数时， $\Psi(x)$可按 $\hat{F}$ 本征函数展开$\Psi(x)=\sum_n c_n\,\psi_n(x)$，测量力学量的结果是$\hat{F}$ 本征值之一，测量结果为λ_n的几率为$|c_n|^2$

(3) 波(态)函数可以完全描述微观粒子的状态

量子力学关于力学量与算符的关系的一个基本假定:

量子力学中表示力学量的算符都是厄密算符, 它们的本征函数组成完全系，当体系处于波函数$\Psi(x)$所描写的状态时，测量力学量F所得的数值必定是算符$\hat{F}$的本征值之一，测得λ_n的几率为$|c_n|^2$

力学量算符的平均值

对于状态$\Psi(x)$，将其按某力学量的本征函数集$\psi_n(x)$展开

$$\Psi(x)=\sum_n c_n\,\psi_n(x) \qquad \psi_n(x)\text{是归一化的}$$

出现本征值λ_n的几率为$|c_n|^2$,则按由几率求平均值的法则

$$\boxed{\langle F\rangle=\sum_n \lambda_n|c_n|^2}$$

上式可改写为

$$\boxed{\langle F\rangle=\int \Psi^*(x)\,\hat{F}\Psi(x)dx=(\Psi,\hat{F}\Psi)}$$

$\Psi(x)$是归一化的

力学量算符的平均值

证明

$$\langle F\rangle=\int\Psi^*(x)\,\hat{F}\Psi(x)dx$$

$$=\sum_{m,n}c_m^*c_n\int\psi_m^*\hat{F}\psi_n dV=\sum_{m,n}c_m^*c_n\lambda_n\int\psi_m^*\psi_n dV=\sum_{m,n}c_m^*c_n\lambda_n\,\delta_{mn}$$

$$=\sum_n\lambda_n|c_n|^2$$

- 如$\Psi(x)$未归一化： $\boxed{\langle F\rangle=\dfrac{\int\Psi^*(x)\hat{F}\Psi(x)dx}{\int\Psi^*(x)\Psi(x)dx}}$

力学量算符的平均值

- 如本征值是连续谱λ

$$\Psi(x)=\int c_\lambda \psi_\lambda(x)d\lambda$$

$$\langle F\rangle=\int \lambda|c_\lambda|^2 d\lambda$$

显然，在任何状态下，厄密算符的平均值都是实数

3.4 The Generalized Statistical Interpretation

If you measure an observable ***Q*(*x*,*p*)** on a particle in the state $\Psi(x,t)$, you get one of the eigenvalues of the hermitian operator

$$\hat{Q}(x, -i\hbar d/dx)$$

If its spectrum is discrete, the probability of getting the particular eigenvalue q_n associated with the orthonormalized eigenfunction $f_n(x)$ is

$$|c_n|^2, \quad \text{where } c_n = \langle f_n | \Psi \rangle$$

If its spectrum is continuous, with real eigenvalue *q(z)* and associated Dirac orthonormalized eigenfunction $f_z(x)$, the probability of getting a result in the range *dz* is

$$|c_n|^2 dz, \quad \text{where} \quad c(z) = \langle f_z | \Psi \rangle$$

Upon measurement, the wave function "collapses" to the corresponding eigen state.

The eigenfunctions of an observable operator are complete, so that wave function can be written as a linear combination of them:

$$\Psi(x,t)=\sum_n c_n f_n(x)$$

Because the eigenfunctions are orthonormal, the coefficients are given by Fourier's trick

$$c_n=\langle f_n|\Psi\rangle=\int f_n^*(x)\Psi(x,t)dx, \Rightarrow \sum_n |c_n|^2=1$$

The expectation value of Q is the sum over all possible outcomes of the eigenvalue times the probability of getting that eigenvalue:

$$\langle Q\rangle = \sum_n q_n |c_n|^2 .$$

Example: measurement of x on a particle in state Ψ, since the eigenfunction is $g_y(x) = \delta(x-y)$ for eigenvalue y, so

$$c(y) = \langle g_y | \Psi \rangle = \int_{-\infty}^{+\infty} \delta(x-y)\Psi(x,t)dx = \Psi(y,t)$$

The probability of getting a result in the range dy is $|\Psi(y,t)|^2 dy$, is precisely the original statistical interpretation.

Example: measurement of momentum p on a particle in state Ψ, since the eigenfunction is

$$f_p(x) = (1/\sqrt{2\pi\hbar})\exp(ipx/\hbar)$$

for eigenvalue p, so

$$c(p) = \langle f_p | \Psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{ipx/\hbar} \Psi(x,t) dx$$

Momentum space wave function, $\Phi(p,t)$.

Inverse Fourier transform.

According to the generalized statistical interpretation, the probability that a measurement of momentum would yield a result in the range dp is

$$|\Phi(p,t)|^2 \, dp$$

Example: A particle of mass m is bound in the delta function well V(x)=-αδ(x). What is the probability that a measurement of its momentum would yield a value greater than $p_0 = m\alpha/\hbar$?

Solution: The wave function is

$$\Psi(x,t) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} e^{-iEt/\hbar}, \quad E = -m\alpha^2/(2\hbar^2)$$

The momentum space wave function is therefore

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \frac{\sqrt{m\alpha}}{\hbar} e^{-iEt/\hbar} \int_{-\infty}^{+\infty} e^{-ipx/\hbar} e^{-m\alpha|x|/\hbar^2} dx = \sqrt{\frac{2}{\pi}} \frac{p_0^{3/2}}{p^2+p_0^2} e^{-iEt/\hbar}$$

The probability is $\frac{2}{\pi} p_0^3 \int_{p_0}^{+\infty} \frac{dp}{\left(p^2+p_0^2\right)^2} = \frac{1}{\pi}\left[\frac{pp_0}{p^2+p_0^2} + \tan^{-1}\left(\frac{p}{p_0}\right)\right]\Bigg|_{p_0}^{\infty} = \frac{1}{4} - \frac{1}{2\pi} = 0.0908$

• 3.6 Dirac Notation

在几何学或经典力学中，常用矢量形式讨论问题而不指明坐标系. 同样，量子力学中描写态和力学量，也可以不用具体表象. 这种描写的方式是狄喇克最先引用的，这样的一套符号就称为狄喇克符号.微观体系的状态可以用一种矢量来表示，它的符号是$|s(t)\rangle$，称为右矢；也可以用另一种矢量来表示，这种矢量的符号是$\langle s(t)|$，称为左矢.

For the state $|\mathcal{S}(t)\rangle$ of a system in quantum mechanics, it is independent with the *bases*.

But it can be expressed in wave function form.

The wave function $\Psi(x,t)$ is actually the coefficient in the expansion of $|\mathcal{S}(t)\rangle$ in the basis of position eigen-functions:

$$\Psi(x,t) = \langle x | \mathcal{S}(t) \rangle,$$

The momentum space wavefunction $\Phi(p,t)$ is the expansion of $|\Psi>$ in the basis of momentum eigenfunctions:

$$\Phi(p,t) = \langle p | \Psi(t) \rangle$$

we could expand $|\Psi>$ in the basis of energy eigenfunctions:

$$c_n(t) = \langle n | \Psi(t) \rangle$$

They are all the same state; the function Ψ and Φ, and the collection of coefficients $\{c_n\}$, contain exactly the same information—they are simple three **different ways of describing the same vector:**

$$\Psi(x,t) = \int \Psi(y,t)\delta(x-y)dy$$

$$= \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}dp$$

$$= \sum c_n e^{-iE_n t/\hbar}\psi_n(x)$$

Operators are linear transformations—they "transform" one vector into another:

$$|\beta\rangle = \hat{Q}|\alpha\rangle$$

Just as vectors are represented, with respect to a particular basis,

$$\langle e_m|\hat{Q}|e_n\rangle \equiv Q_{mn}$$

Then

$$|\beta\rangle = \hat{Q}|\alpha\rangle \Rightarrow \sum_n b_n|e_n\rangle = \sum_n a_n\hat{Q}|e_n\rangle$$

$$\Rightarrow \sum_n b_n\langle e_m||e_n\rangle = \sum_n a_n\langle e_m|\hat{Q}|e_n\rangle$$

$$\Rightarrow b_m = \sum_n Q_{mn}a_n$$

Example: Imagine a system in which there are just two linearly independent states:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The most general state is a normalized linear combination:

$$|\mathcal{S}\rangle = a|1\rangle + b|2\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \text{ with} |a|^2 + |b|^2 = 1.$$

The Hamiltonian can be expressed as a (hermitian) matrix; suppose it has the specific form

$$H = \begin{pmatrix} h & g \\ g & h \end{pmatrix}$$

where g and h are real constants. If the system starts out (t=0) in state |1>, what is its state at time t?

Solution: The TDSE says $$i\hbar\frac{d}{dt}|\mathcal{S}\rangle = H|\mathcal{S}\rangle$$

as always, we begin by solving the TISE:

$$H|\mathcal{S}\rangle = E|\mathcal{S}\rangle;$$

i.e., find the eigenvectors and eigenvalues of H. The characteristic equation determines the eigenvalues:

$$\det\begin{pmatrix} h-E & g \\ g & h-E \end{pmatrix} = 0 \Rightarrow E_{\pm} = h \pm g$$

Evidently the allowed energies are $(h+g)$ and $(h-g)$. To determine the eigenvectors, we write

$$\begin{pmatrix} h & g \\ g & h \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (h \pm g)\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Rightarrow h\alpha + g\beta = (h \pm g)\alpha \Rightarrow \beta = \pm\alpha$$

so the normalized eigenvectors are

$$|\chi_\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}.$$

Next we **expand the initial state as a linear combination of eigenvectors** of the hamiltonian:

$$|\chi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(|\chi_+\rangle + |\chi_-\rangle\right).$$

Finally, we tack on the standard time-dependence $\exp(-\frac{iE_n t}{\hbar})$

$$\left|\mathcal{S}(t)\right\rangle = \frac{1}{\sqrt{2}}\left(e^{-i(h+g)t/\hbar}\left|\mathcal{S}_+\right\rangle + e^{-i(h-g)t/\hbar}\left|\mathcal{S}_-\right\rangle\right)$$

$$= \frac{1}{2}e^{-iht/\hbar}\left(e^{-igt/\hbar}\begin{pmatrix}1\\1\end{pmatrix} + e^{igt/\hbar}\begin{pmatrix}1\\-1\end{pmatrix}\right)$$

$$= \frac{1}{2}e^{-iht/\hbar}\begin{pmatrix}e^{-igt/\hbar}+e^{igt/\hbar}\\ e^{-igt/\hbar}-e^{igt/\hbar}\end{pmatrix} = e^{-iht/\hbar}\begin{pmatrix}\cos(gt/\hbar)\\ -i\sin(gt/\hbar)\end{pmatrix}.$$

$$H = \begin{pmatrix}h & g\\ g & h\end{pmatrix}$$

end

Dirac chops the bracket notation for the inner product, $\langle\alpha|\beta\rangle$, into two pieces, which he called bra, $\langle\alpha|$ and ket $|\beta\rangle$. In a function space, the bra can be thought of as an instruction to integrate:

$$\langle f| = \int f^*[\cdots]dx$$

In a finite-dimensional vector space,

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \langle\alpha| = \begin{pmatrix} a_1^* & a_2^* & \cdots & a_n^* \end{pmatrix}$$

The collection of all bras constitutes another vector space—**dual space.**

The license to treat bras as separate entities in their own right allows for some powerful and pretty notation. For example, if |α> is a normalized vector, the operator

$$\hat{P} \equiv |\alpha\rangle\langle\alpha|$$

picks out the portion of any other vector that "lies along" |α>

$$\hat{P}|\beta\rangle = \langle\alpha|\beta\rangle|\alpha\rangle;$$

We call it **the projection operator** onto the 1D subspace spanned by |α>. If {|e_n>} is a discrete orthonormal basis,

$$\langle e_m|e_n\rangle = \delta_{mn}, \quad \text{then } \sum_{n}|e_n\rangle\langle e_n| = 1$$

if we let this operator act on any vector |α>, we recover the expansion of |α> in the $\{|e_n>\}$ basis

$$\sum_n |e_n\rangle\langle e_n|\alpha\rangle = |\alpha\rangle$$

Similarly, if $\{|e_n>\}$ is a Dirac orthonormal basis,

$$\langle e_z|e_{z'}\rangle = \delta(z-z') \quad \text{then} \quad \int |e_z\rangle\langle e_z| dz = 1$$

For example, the one qubit NOT gate corresponds to the operator $|0\rangle\langle 1| + |1\rangle\langle 0|$

e.g.

$$
\begin{aligned}
&\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right)\left(|0\rangle\right) \\
&= |0\rangle\langle 1||0\rangle + |1\rangle\langle 0||0\rangle \\
&= |0\rangle\langle 1|0\rangle + |1\rangle\langle 0|0\rangle \\
&= 0|0\rangle + 1|1\rangle \\
&= |1\rangle
\end{aligned}
$$

The NOT gate is a 1-qubit unitary operation.

The corresponding expressions in real space and Dirac notation

$$\int \psi^*(x)\varphi(x)dx \qquad \langle \psi | \varphi \rangle$$

$$\hat{F}(x,-i\hbar\frac{\partial}{\partial x})\Psi(x,t) = \Phi(x,t) \qquad \langle x|\hat{F}|\Psi\rangle = \langle x|\Phi\rangle \quad \textbf{or} \quad \hat{F}|\Psi\rangle = |\Phi\rangle$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}(x,-i\hbar\frac{\partial}{\partial x})\Psi(x,t) \qquad i\hbar\frac{\partial}{\partial t}\langle x|\Psi\rangle = \langle x|\hat{H}|\Psi\rangle$$

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

$$\hat{H}(x,-i\hbar\frac{\partial}{\partial x})u_n(x) = E_n u_n(x) \qquad \hat{H}|n\rangle = E_n|n\rangle$$

$$\int u_n^*(x)u_m(x)dx = \delta_{nm}$$

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

$$\int u_{\lambda'}^*(x)u_\lambda(x)dx = \delta(\lambda' - \lambda)$$

$$\langle\lambda'|\lambda\rangle = \delta(\lambda' - \lambda)$$

$$\int u_\lambda^*(x')u_\lambda(x)d\lambda = \delta(x' - x)$$

$$\int d\lambda|\lambda\rangle\langle\lambda| = 1$$

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

$$\sum_n |n\rangle\langle n| = 1$$

$$\Psi(x) = \sum_n a_n u_n(x)$$

$$|\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle$$

$$a_n = \int u_n^*(x)\Psi(x)dx$$

$$\langle n|\Psi\rangle = \int dx\langle n|x\rangle\langle x|\Psi\rangle$$

- **3.5 The Uncertainty Principle**

不确定性

在自由粒子问题中我们看到， $|p\rangle$是能量和动量的共同本征态：

$$H|p\rangle = \frac{P}{2m}\,p|p\rangle = \frac{p^2}{2m}|p\rangle,$$

但【有共同本征态】不等于【每个本征态都一样】，如：

$$H(|p\rangle + |-p\rangle) = \frac{P}{2m}(p|p\rangle - p|-p\rangle) = \frac{p^2}{2m}(|p\rangle + |-p\rangle),$$
$$P(|p\rangle + |-p\rangle) = p|p\rangle - p|-p\rangle \neq c(|p\rangle + |-p\rangle).$$

反过来，如果两个力学量算符不对易，则一般而言没有**共同本征态**，即不能同时有**确定的取值**。如

$$X|p\rangle = X\int_{-\infty}^{+\infty}|x\rangle\langle x|p\rangle dx = \int_{-\infty}^{+\infty}x|x\rangle\langle x|p\rangle dx \neq c|p\rangle$$

也就是**对一个力学量的本征态可以是其它力学量的叠加态**这一点的体现。

怎么衡量有多不确定呢？显然，如果确定的话，那么期望值就等于每次测量的取值：

$$\langle a_n|A|an\rangle = an,$$

于是想到可以用如下算符自然地衡量A偏离期望值的程度：

$$A - \langle A\rangle I\,,$$

但是并没有这么简单，如果单纯地求这个**偏差算符**的期望值会发现结果是平庸的：

$$\langle\psi|A-\langle A\rangle I|\psi\rangle=\langle\psi|A|\psi\rangle-\langle A\rangle\langle\psi|I|\psi\rangle=\langle A\rangle-\langle A\rangle=0,$$

这可以理解为期望值两侧正负偏差平均相抵，为了避免这种相抵，我们可以求它平方的期望值：

$$\langle(A-\langle A\rangle)^2\rangle=\langle A^2-2\langle A\rangle A+\langle A\rangle^2\rangle=\langle A^2\rangle-2\langle A\rangle^2+\langle A\rangle^2=\langle A^2\rangle-\langle A\rangle^2,$$

即A平方的期望减去期望的平方，统计学中称为**方差。**

我们将其开方以得到和A同量纲的量：

$$\sigma_A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2},$$

称为**标准差**，即，**不确定性。**

容易验证，当且仅当在A的本征态上计算时，σA才等于零，在其它态上非零，可见其确实衡量了A的不确定的程度。

不确定性关系

海森堡最早发现位置和动量的不确定性之间有一定的关系，

$$\sigma_X \sigma_P \geq \hbar/2,$$

一般而言：两个力学量 A 和 B 的不确定性的乘积有一个下限，这个下限和它们的对易子的期望的模有关：

$$\sigma_A \sigma_B \geq 1/2|\langle [A,B] \rangle|.$$

将正则对易关系$[X,P]=i\hbar I$代入即可得到位置与动量的不确定关系。

可以证明，对于有限维的力学量算符，其对易子不可能是$i\hbar$这样的常数（常数倍的单位算符），只有像位置、动量这样取值连续的力学量才可以，一般来说对易子不是常数，故**不确定性乘积的下限是可变的。**

如对自由粒子的位置和能量：$[X,H]=[X,P^2/2m]=XP^2/2m-P^2/2mX$,

利用$XP-PX=i\hbar I$有 $[X,H]=i\hbar P/m$,

对易子正比于动量，则位置和能量的不确定性关系为：

$$\sigma_X\sigma_H \geq \frac{\hbar}{2m}\langle P\rangle.$$

于是对于不同平均动量的态，位置和能量的不确定性下限是不同的。

不确定性的物理意义

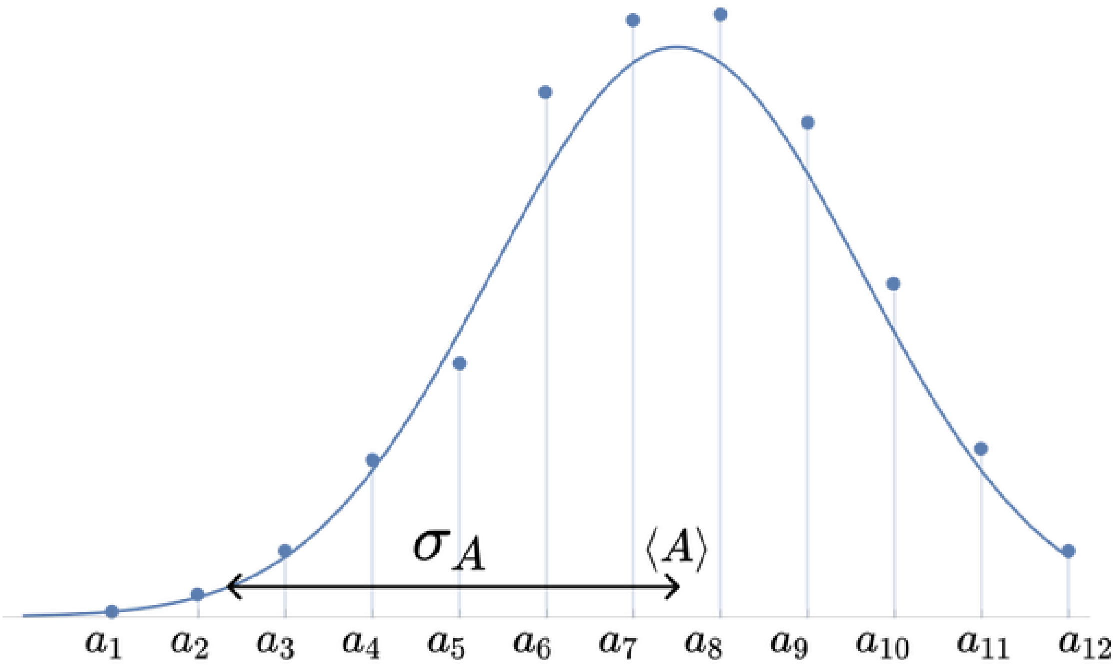
上文定义的不确定性的物理意义是很清楚的。不确定性，进而不确定性关系是源于态叠加原理，基于态矢量和算符的量子力学理论结构的 **必然结果**。不确定性原理与测量行为无关，而是态矢量在不同表象中的“投影”带来的固有的概率分布。

为了实际观测不确定性，以及更早引入的期望值，我们需要引入**系综**（ensemble）。理论上，只要得知了系统的态$|\psi\rangle$，那任意力学量A的$\langle A\rangle,\sigma_A$都容易由定义算出，但实验中我们往往不知道$|\psi\rangle$。如果测量系统，我们能确定的只是测量后的态是什么，而**无法得知测量前的态**——除非我们准备大量都由$|\psi\rangle$描述的系统，称为**系综**——尽管我们不知道$|\psi\rangle$具体是什么，但**确实可以使系统都制备到同一个未知的初态。**

（【注】这种系综称为**纯系综**。还有一种系综称为**混合系综**，其中系统不是由同一个态矢量$|\psi\rangle$描述，而是由**同一组**可能的态矢量$\{|\psi_1\rangle,\cdots,|\psi_N\rangle\}$和一组概率$\{p_1,\cdots,p_N\}$描述，每个系统都有概率由其中一个态矢量描述。这里说的概率是经典概率，如我们可以通过抛硬币来决定每个系统到底是制备成$|\psi_1\rangle$还是$|\psi_2\rangle$。这也可以说是一种叠加，但没有相干性，故也称为非相干叠加。）

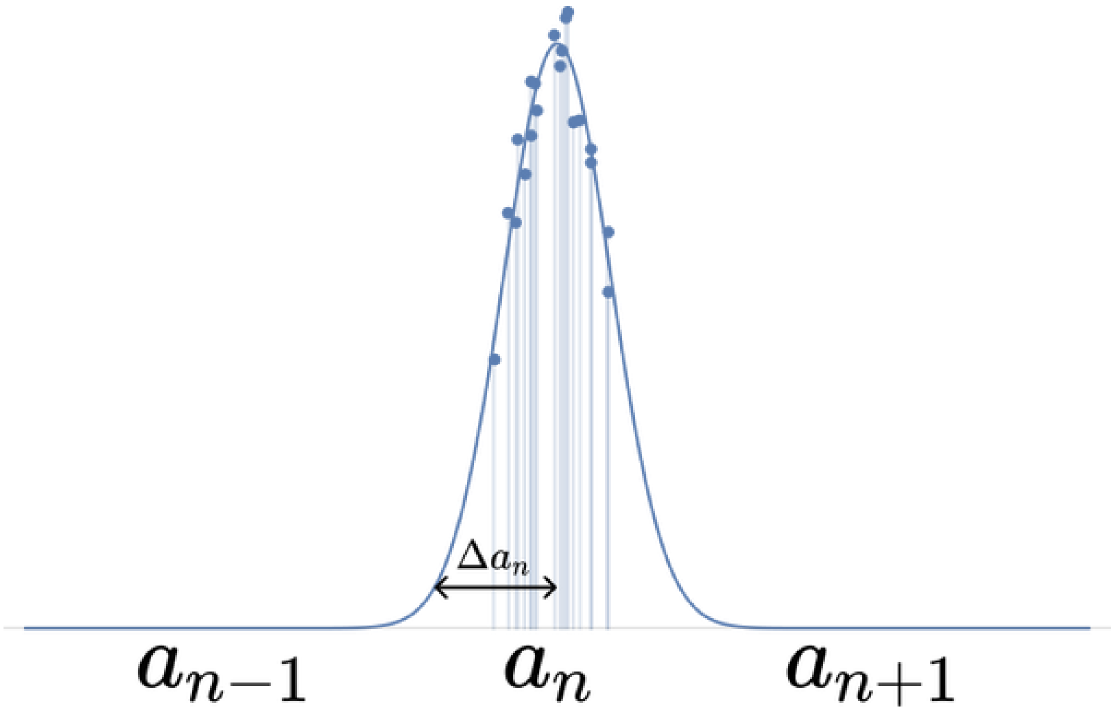
系综中每个系统都随机地投影，统计其中各个测量结果的**频率**，我们就能逐渐逼近理论概率$\langle a_n|\psi\rangle$，进而得到$\langle A\rangle,\sigma_A$。量子力学中所说的重复测量往往都是指对系综的测量。

于是，**不确定性在理论上是量子态的内禀属性，在实验上则是系综的属性**。由于力学量之间的不对易性，一个态**不可能是所有力学量的共同本征态**，它必然对某些力学量是叠加态，也就伴随着相应的内禀不确定性。



本征值、期望值、不确定性示意图。图中曲线由理论概率连成，散点为实验测得频率。

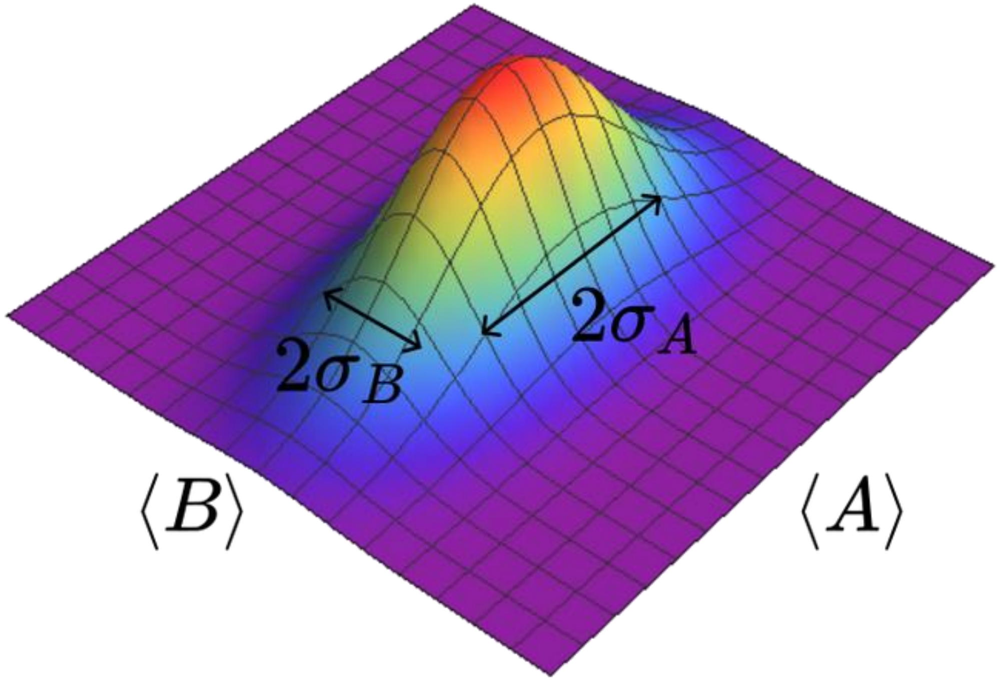
我们应当**将这种内禀不确定性与实验误差区分开来**，图中可以看到，不确定性体现为理论概率曲线的“宽度”。而实验误差在这里体现为什么呢？设系综中有些系统投影到$|a_n\rangle$，理论上我们的测量结果就是a_n，但误差使得这些投影到$|a_n\rangle$的系统，有些在仪器上输出值比a_n大一点，有些则小一点——实验测量结果落在以a_n为中心的一个区间。最终，实验$\langle A\rangle$实验和理论值也就略有不同。



测量本征值a_n的误差示意图，上图中一个点的放大。若误差Δa_n太大，则a_n与a_{n-1}，a_{n+1}将无法区分开，测量也不再能看成理想的投影测量。

对不对易力学量A,B，右图直观地体现了不确定性关系。当不确定性乘积（粗略地说，曲面下方面积）相对于所关心的尺度很小时，就可以近似认为A,B同时确定，取值即为期望值⟨A⟩,⟨B⟩。如对加速器中的粒子，我们之所以可以像经典质点一样研究其运动轨迹就是因为不确定性小于分辨能力。

注】当然，还需要环境相互作用来阻止不确定性无限增大。



不确定性关系示意图。不确定性关系禁止我们将图中曲面缩小为一个只占据一点的尖峰。

不确定性关系的推导

我们需要引入一个不等式，<u>施瓦茨不等式</u>：

$$\langle a|a\rangle\langle b|b\rangle \geq |\langle a|b\rangle|^2,$$

对此我们不作证明，你可以类比欧氏矢量来理解，对欧氏矢量有：

$$|\boldsymbol{a}|^2|\boldsymbol{b}|^2 \geq |\boldsymbol{a}\cdot\boldsymbol{b}|^2,$$

当且仅当$\boldsymbol{a}$和$\boldsymbol{b}$平行才取等号。

令$|a\rangle = (A - \langle A\rangle)|\psi\rangle$，$|b\rangle = (B - \langle B\rangle)|\psi\rangle$，

由施瓦茨不等式：$\sigma_A\sigma_B = \sqrt{\langle a|a\rangle\langle b|b\rangle} \geq \sqrt{|\langle a|b\rangle|^2} = |\langle a|b\rangle|$,

而

$$|\langle a|b\rangle| = \sqrt{(\mathrm{Re}\langle a|b\rangle)^2 + (\mathrm{Im}\langle a|b\rangle)^2} \geq |\mathrm{Im}|\langle a|b\rangle| = \frac{1}{2}|\langle a|b\rangle - \langle b|a\rangle|,$$

接下来计算$\langle a|b\rangle$:

$$\langle a|b\rangle = \langle\psi|AB - \langle A\rangle B - \langle B\rangle A + \langle A\rangle\langle B\rangle|\psi\rangle = \langle\psi|AB|\psi\rangle - \langle\psi|A|\psi\rangle\langle\psi|B|\psi\rangle,$$

$$\langle b|a\rangle = \langle a|b\rangle^* = \langle\psi|BA|\psi\rangle - \langle\psi|A|\psi\rangle\langle\psi|B|\psi\rangle.$$

代入上面即证得不确定性关系:

$$\sigma_A\sigma_B \geq 1/2\langle|[A,B]|\rangle.$$

This is the **generalized uncertainty principle**.

- There is an "uncertainty principle" for every pair of observables whose operators do not commute. –incompatible observables.
- Incompatible observables do not have shared eigenfunctions.
- compatible (commuting) observables do admit complete sets of simultaneous eigenfunctions.

Example:

$$\boxed{\sigma_A^2\sigma_B^2 \ge \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2}$$

Heisenberg uncertainty principle : $\begin{cases} \hat{A} = x \\ \hat{B} = \hat{p} = -i\hbar\dfrac{d}{dx} \end{cases}$

then $[\hat{x},\hat{p}]f(x) = x(-i\hbar)\dfrac{df}{dx} - (-i\hbar)\dfrac{d}{dx}(xf)$

$$= -i\hbar x\frac{df}{dx} + i\hbar x\frac{df}{dx} + i\hbar f$$

$$= i\hbar f$$

so $[\hat{x},\hat{p}] = i\hbar$

$$\sigma_x^2\sigma_p^2 \ge \left(\frac{1}{2i}i\hbar\right)^2 = \left(\frac{\hbar}{2}\right)^2 \Rightarrow \boxed{\sigma_x\sigma_p \ge \frac{\hbar}{2}}$$

➢ Energy-time uncertainty principle

for the expectation value of an observable $Q(x, p, t)$

$$\frac{d}{dt}\langle \hat{Q}\rangle = \frac{d}{dt}\langle \Psi \mid \hat{Q}\Psi\rangle = \langle \frac{\partial \Psi}{\partial t} \mid \hat{Q}\Psi\rangle + \langle \Psi \mid \frac{\partial \hat{Q}}{\partial t}\Psi\rangle + \langle \Psi \mid \hat{Q}\frac{\partial \Psi}{\partial t}\rangle$$

by Schrödinger equation $\quad i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi$

$$\Rightarrow \quad \frac{d}{dt}\langle \hat{Q}\rangle = \langle -\frac{i}{\hbar}\hat{H}\Psi \mid \hat{Q}\Psi\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle + \langle \Psi \mid (-\frac{i}{\hbar})\hat{Q}\hat{H}\Psi\rangle$$

$$= \frac{i}{\hbar}\langle \hat{H}\Psi \mid \hat{Q}\Psi\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle - \frac{i}{\hbar}\langle \Psi \mid \hat{Q}\hat{H}\Psi\rangle$$

$$= \frac{i}{\hbar}\langle \Psi \mid \hat{H}\hat{Q}\Psi\rangle - \frac{i}{\hbar}\langle \Psi \mid \hat{Q}\hat{H}\Psi\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle$$

$$= \frac{i}{\hbar}\langle [\hat{H},\hat{Q}]\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle$$

$$\Rightarrow \quad \langle [\hat{H},\hat{Q}]\rangle = \frac{\hbar}{i}\frac{d}{dt}\langle \hat{Q}\rangle - \frac{\hbar}{i}\langle \frac{\partial \hat{Q}}{\partial t}\rangle$$

typical case: operator does not depend explicitly on time,

$$\text{so} \quad \sigma_H^2\sigma_Q^2 \geq \left(\frac{1}{2i}\langle [\hat{H},\hat{Q}]\rangle\right)^2 = \left(\frac{1}{2i}\frac{\hbar}{i}\frac{d\langle \hat{Q}\rangle}{dt}\right)^2 = \left(\frac{\hbar}{2}\right)^2\left(\frac{d\langle \hat{Q}\rangle}{dt}\right)^2$$

$$\Rightarrow \quad \sigma_H\sigma_Q \geq \frac{\hbar}{2}\left|\frac{d\langle \hat{Q}\rangle}{dt}\right|$$

define $\Delta E \equiv \sigma_H$, $\Delta t \equiv \dfrac{\sigma_Q}{\left| d\langle \hat{Q} \rangle / dt \right|}$

then $\Delta E \Delta t \geq \dfrac{\hbar}{2}$ …….. is **energy-time uncertainty principle**

- *Δt* represents the amount of time it takes the expectation value of *Q* to *change by one standard deviation.*
- In particular, *Δt* depends entirely on what observable you care to look at—the change might be rapid for one observable and slow for another.
- If ΔE is samll, then the rate of change of all observables must very gradual. If any observables changes rapidly, the "uncertainty" in the energy must be large.

The uncertainty relations of energy and time for a particle

It is well known that the atomic emission spectral lines are not infinitely narrow – this would correspond to an uncertainty in the radiation of a quantum of energy of $\Delta E = 0$. The spectral lines that are observed in experiments have a so-called natural linewidth $\Delta\omega$. The width of this spectral line is determined by the spread of the photon's energy values $\Delta E = \hbar\omega$ with respect to the mean value that characterizes the center of the line $E = \hbar\omega$. This width is related to the lifetime of an atom in the excited state, Δt, by the uncertainty relation

$$\Delta E\Delta t = \hbar\omega\Delta t \approx h, \text{ i.e., } \Delta\omega\Delta t \approx 2\pi.$$

The uncertainty relations of energy and time for a particle

By experimentally measuring the natural linewidth we can find the lifetime of an atom in the corresponding excited state.

The natural linewidth which corresponds to the visible range of emission of atoms is of the order of $\Delta\omega \sim 10^{8}\text{s}^{-1}$.

Therefore, the atomic lifetime in the excited state is about $\Delta t \sim 10^{-8}\text{s}$.

The uncertainty relations of energy and time for a particle

Taking into account that the frequency in the visible range is about $\omega \approx 4 \times 10^{15} s^{-1}$, we can find the relative width of the emission spectral line: $\Delta\omega/\omega \approx 2.5 \times 10^{-8}$.

Note that in the ground state, i.e., in the non-excited state, stable (light) atoms can have indefinitely long lifetimes,

i.e., in this state the lifetime of an atom $\tau \rightarrow \infty$, while the width of the energy level that corresponds to the ground state $\Delta E \rightarrow 0$.

Problem 3.36 **Extended uncertainty principle.** The generalized uncertainty principle states that $\sigma_A^2\sigma_B^2 \geq \frac{1}{4}\langle C\rangle^2$, where $\hat{C} \equiv -i[\hat{A},\hat{B}]$.

(a) Show that it can be strengthened to read $\sigma_A^2\sigma_B^2 \geq \frac{1}{4}(\langle C\rangle^2 + \langle D\rangle^2)$, where $\hat{D} \equiv \hat{A}\hat{B} + \hat{B}\hat{A} - 2\langle A\rangle\langle B\rangle$

(a) For any observable A, we have

$$\sigma_A^2 = \langle(\hat{A} - \langle A\rangle)\Psi|(\hat{A} - \langle A\rangle)\Psi\rangle = \langle f|f\rangle, \quad \sigma_B^2 = \langle g|g\rangle, \quad \text{where } g \equiv (\hat{B} - \langle B\rangle)\Psi.$$

(invoking the Schwarz inequality $\sigma_A^2\sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2$.

for any complex number z,

$$|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 = \left[\frac{1}{2}(z+z^*)\right]^2 + \left[\frac{1}{2i}(z-z^*)\right]^2$$

$$\sigma_A^2\sigma_B^2 \geq \left[\frac{1}{2}\left(\langle f|g\rangle + \langle g|f\rangle\right)\right]^2 + \left[\frac{1}{2i}\left(\langle f|g\rangle - \langle g|f\rangle\right)\right]^2.$$

You can find, <*f*|*g*>= <AB> -<A><B>, <*g*|*f*>= <BA>-<A><B>,

$$\langle f|g\rangle - \langle g|f\rangle = \langle[\hat{A}, \hat{B}]\rangle \qquad \langle f|g\rangle + \langle g|f\rangle = \langle D\rangle.$$

$$\text{So } \sigma_A^2\sigma_B^2 \geq \frac{1}{4}\left(\langle D\rangle^2 + \langle C\rangle^2\right).$$

两个力学量可同时确定的条件

算符的对易关系

共同本征态函数

测不准关系

$$\hat{K}=0$$

$$[\hat{A},\hat{B}]=i\hat{K}$$

$$\hat{A}\Phi_n=\lambda_n\Phi_n\,,$$

$$\hat{B}\Phi_n=\mu_n\Phi_n$$

$$\langle(\Delta\hat{A})^2\rangle\cdot\langle(\Delta\hat{B})^2\rangle\geq\frac{\langle\hat{K}\rangle^2}{4}$$

算符的对易关系

- 如果两个算符在乘积中可以交换位置,我们称为它们可以对易,反之,不对易。$\hat{A}\hat{B}$和$\hat{B}\hat{A}$的差定义对易关系（第16讲我们已经有初步印象）：

$$\boxed{[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}}$$

显然

$$[\hat{A},\hat{A}] = 0, \qquad [\hat{A},C] = 0, \qquad [C\hat{A},\hat{B}] = [\hat{A},C\hat{B}] = C[\hat{A},\hat{B}],$$

$$[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$$

算符的对易关系

对易关系性质

$$[\hat{A},\hat{B}]=-[\hat{B},\hat{A}]$$

$$[\hat{A},\hat{B}\hat{C}]=\hat{B}[\hat{A},\hat{C}]+[\hat{A},\hat{B}]\hat{C}$$

$$[\hat{A}\hat{B},\hat{C}]=\hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B}$$

$$[\hat{\boldsymbol{A}}\times\hat{\boldsymbol{B}},\hat{C}]=\hat{\boldsymbol{A}}\times[\hat{\boldsymbol{B}},\hat{C}]+[\hat{\boldsymbol{A}},\hat{C}]\times\hat{\boldsymbol{B}}$$

算符具有共同本征态函数的条件

如两算符$\hat{A},\hat{B}$满足 $[\hat{A},\hat{B}]=0$ 称$\hat{A},\hat{B}$对易

定理： 如果两算符$\hat{A},\hat{B}$有一组共同本征函数Φ_n，而且Φ_n组成完全系，则$\hat{A},\hat{B}$对易

证

$$\hat{A}\Phi_n=\lambda_n\Phi_n,\ \hat{B}\Phi_n=\mu_n\Phi_n$$

$$(\hat{A}\hat{B}-\hat{B}\hat{A})\Phi_n=\lambda_n\mu_n\Phi_n-\mu_n\lambda_n\Phi_n=0$$

设Ψ是任一波函数, $\Psi=\sum_n a_n\Phi_n$

$$(\hat{A}\hat{B}-\hat{B}\hat{A})\Psi=\sum_n a_n(\hat{A}\hat{B}-\hat{B}\hat{A})\Phi_n=0$$

算符具有共同本征态函数的条件

所以

$$\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)=0$$

逆定理: 如果两个算符对易，则这两个算符有组成完全系的共同本征函数。上述定理可推广到两个以上算符的情况。

共同本征波函数系
不确定关系

关于共同本征态函数的讨论

例 $[\hat{L}^2, \hat{L}_z] = 0$, $\hat{L}^2, \hat{L}_z$的共同本征函数完全集是$Y_{lm}(\theta, \varphi)$

$\hat{p}_x, \hat{p}_y, \hat{p}_z$相互对易，它们有共同本征函数$\Psi_{\boldsymbol{p}}(\boldsymbol{r}) = C\exp\left(\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}\right)$

- 如两算符$\hat{A}, \hat{B}$对易，二者在共同本征函数状态是同时完全确定的，
- 如果两算符$\hat{A}, \hat{B}$不对易，二者没有共同本征函数，如果$\hat{A}\Phi_n = \lambda_n\Phi_n$,$\hat{B}\varphi_n = \mu_n\varphi_n$，那我们可以把每一个$\Phi_n$用$\{\varphi_n\}$展开

$$\boxed{\Phi_n = \sum_i C_{ni}\varphi_i}$$

在Φ_n态力学量 $\hat{B}$只能有可能只而无确定值，反之亦然。

关于共同本征态函数的讨论

波函数无法直接测量，要确定系统状态，可以通过测量力学量A,B,C来解决，这些力学量算符都要两两对易，找到它们的共同本征函数Ψ_{ABC}，而Ψ_{ABC}是非简并的，这样力学量A,B,C确定后，系统的状态就可确定。

即：通过力学量A,B,C的测量，提供确定状态波函数Ψ_{ABC}的完备条件。这一套力学量称为“力学量的完全集合”

关于共同本征态函数的讨论

力学量的完全集合是可以同时测量的，对其的测量——“完全测量”。

完全集合中力学量的数目在经典物理中为自由度的2倍，在量子力学中与自由度数目相符。

从对易关系可以看出，普朗克常数在力学量对易关系中占有重要地位。体系微观规律与宏观规律之间差异，如$\hbar$在所讨论问题中可略去，则坐标，动量，角动量之间都对易，这些力学量同时有确定值，微观体系就过渡到宏观体系。

不确定关系再举例

例 通过测不准原理关系说明线性谐振子的零点能

解 振子的平均能量是

$$\langle E\rangle=\frac{\langle p\rangle^2}{2m}+\frac{1}{2}m\omega^2\langle x\rangle^2 \qquad \langle\hat{x}\rangle=0, \qquad \langle\hat{p}\rangle=0$$

$$\because \langle(\Delta\hat{x})^2\rangle=\langle\hat{x}^2\rangle-\langle\hat{x}\rangle^2=\langle\hat{x}^2\rangle$$

$$\langle(\Delta\hat{p})^2\rangle=\langle\hat{p}^2\rangle$$

$$\therefore \langle E\rangle=\frac{\langle(\Delta\hat{p})^2\rangle}{2m}+\frac{1}{2}m\omega^2\langle(\Delta\hat{x})^2\rangle$$

不确定关系再举例

- $\langle(\Delta\hat{x})^2\rangle$ 和$\langle(\Delta\hat{p})^2\rangle$的不确定关系取等号

$$\langle(\Delta\hat{p}_x)^2\rangle = \frac{\hbar^2}{4\langle(\Delta\hat{x})^2\rangle}$$

$$\langle E\rangle = \frac{\hbar^2}{8m}\frac{1}{\langle(\Delta\hat{x})^2\rangle} + \frac{1}{2}m\omega^2\langle(\Delta\hat{x})^2\rangle = (\cdots)^2 + \frac{1}{2}\hbar\omega$$

- 得出的最小值$\frac{1}{2}\hbar\omega$。

不确定关系是量子力学中的基本关系，它反映了微观粒子波粒二象性。

Summary

- **3.1 Hilbert space** $\langle f \mid g \rangle = \int_a^b f^*(x) g(x) dx$

- **3.2 Observables** $\langle Q \rangle = \langle Q \rangle^*$ $\hat{Q}\Psi = q\Psi$

- **3.3 Eigenfunctions of a Hermitian Opertor**

$$\langle \hat{\mathbf{A}} \rangle = \int \Psi^* \hat{\mathbf{A}} \Psi d\tau = \sum_{j=1}^{N} |c_j|^2 \lambda_j$$

- **3.4 The Generalized Statistical Interpretation**

$$|c_n|^2 dz, \quad \text{where} \quad c(z) = \langle f_z | \Psi \rangle$$

- **3.5 The Uncertainty Principle** $\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2$

- **3.6 Dirac Notation** $\hat{P} \equiv |\alpha\rangle\langle\alpha|$