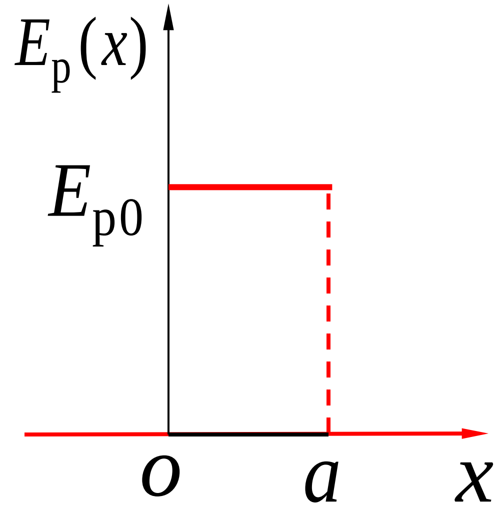
四　隧道效应



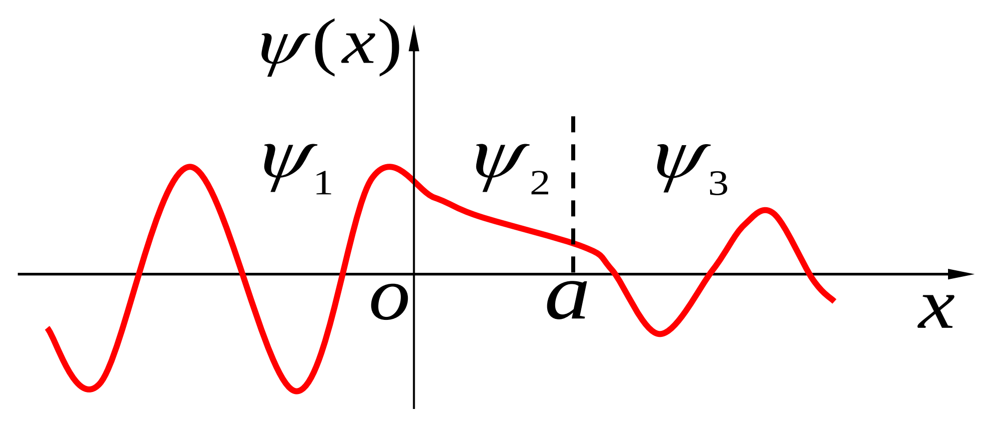
一维方势垒

$$E_p(x) = \begin{cases} 0, & x < 0, x > a \\ E_{p0}, & 0 \le x \le a \end{cases}$$

粒子的能量　$E < E_{p0}$

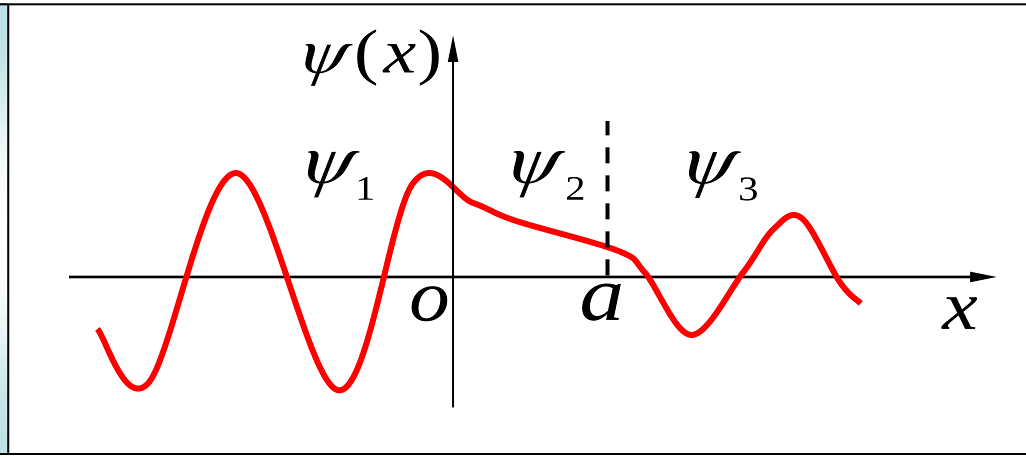
隧道效应

从左方射入的粒子，在各区域内的波函数



隧道效应

从左方射入的粒子，在各区域内的波函数



当粒子能量 $E < E_{p0}$ 时，从经典理论来看，粒子不可能穿过进入 $x > a$ 的区域。但用量子力学分析，粒子有一定概率贯穿势垒，事实表明，量子力学是正确的。

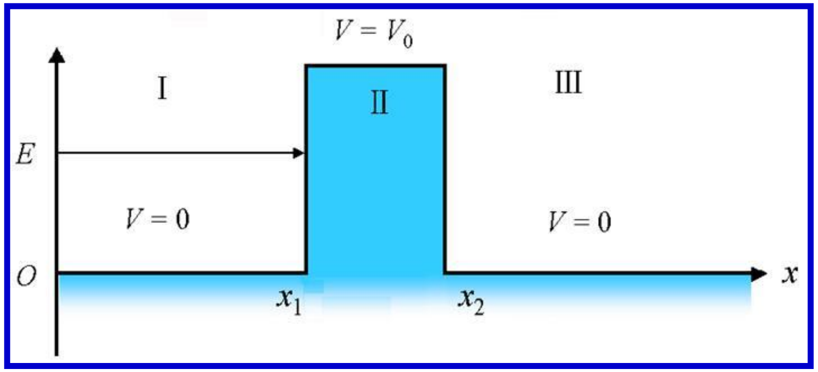
粒子的能量虽不足以超越势垒，但在势垒中似乎有一个隧道，能使少量粒子穿过而进入 $x > a$ 的区域，此现象人们形象地称为隧道效应。

隧道效应的本质：来源于微观粒子的波粒二象性。

势垒 势垒贯穿

1. 势垒 (Potential barrier)

$$V(x)=\begin{cases}0 & x<x_1,\ x>x_2\\ V_0 & x_1\le x\le x_2\end{cases}$$



2. 定态薛定谔方程

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r})\right]\psi(\vec{r})=E\psi(\vec{r})$$

3. 分区求通解

I区 $x<x_1$: $$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x)=E\psi(x)$$

令 $k^2=\dfrac{2mE}{\hbar^2}$ 得 $\psi''(x)+k^2\psi(x)=0$

$$\psi_{\mathrm{I}}(x)=A\sin(kx+\alpha)$$

II 区 $x_1 < x < x_2$:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V_0\right]\psi(x)=E\psi(x)$$

令 $\lambda^2=\frac{2m}{\hbar^2}(V_0-E)$ 得 $\psi''(x)-\lambda^2\psi(x)=0$

$$\psi_{\mathrm{II}}(x)=Be^{\lambda x}+Ce^{-\lambda x}$$

I区域出现粒子的几率一定比III大 → $B=0$

即 $\psi_{\mathrm{II}}(x)=Ce^{-\lambda x}$

III区 $x > x_2$: 与I区情况类似

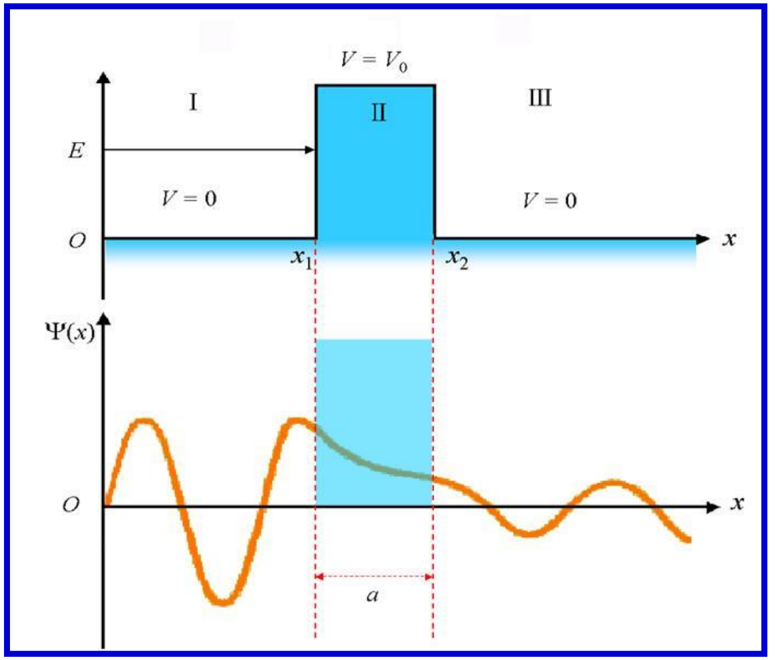
$$\psi_{\mathrm{III}}(x)=D\sin(kx+\beta) \qquad \psi_{\mathrm{III}}(x)\neq 0$$

$x < x_1$内的粒子可以通过势垒区进入$x > x_2$区域

4. 势垒贯穿

穿透势垒的几率

$$p=\frac{|\psi_{\mathrm{III}}(x_2)|^2}{|\psi_{\mathrm{I}}(x_1)|^2}$$



根据波函数的连续性

$$p=\frac{|\psi_{\mathrm{III}}(x_2)|^2}{|\psi_{\mathrm{I}}(x_1)|^2}=\frac{|\psi_{\mathrm{II}}(x_2)|^2}{|\psi_{\mathrm{II}}(x_1)|^2}$$

$$=\frac{C^2e^{-2\lambda x_2}}{C^2e^{-2\lambda x_1}}=e^{-2\lambda(x_2-x_1)}=e^{-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}}$$

① 势垒厚度a越大, 粒子通过的几率越小.

② 势垒高度V_0超过粒子能量E越大, 粒子穿透势垒的几率越小.

怎样理解粒子通过势垒区?

经典物理：从能量守恒的角度看是不可能的。

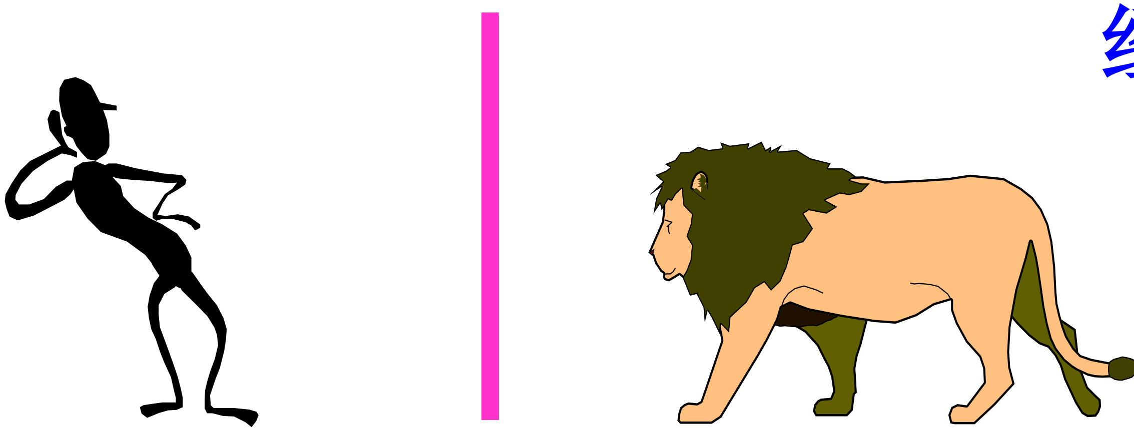
量子物理：粒子有波动性，遵从不确定关系，

只要势垒区宽度$\Delta x = a$不是无限大，粒子能量就有不确定量ΔE。

$$E = \frac{p^2}{2m} \rightarrow \Delta E = \frac{2p\Delta p}{2m} = \frac{p\Delta p}{m}$$

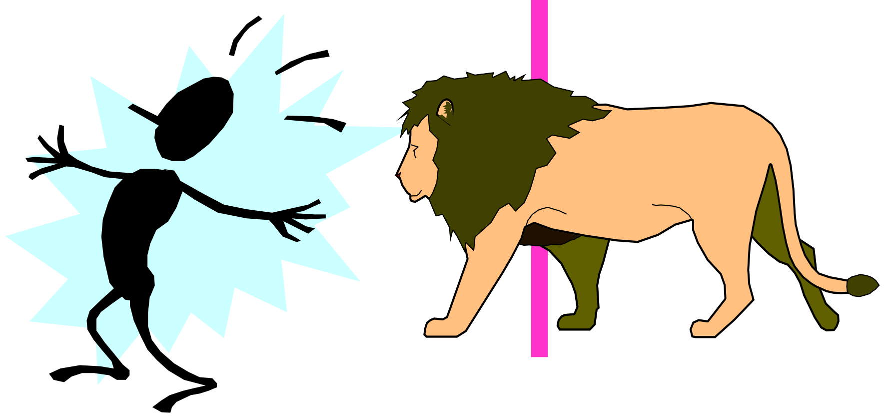
$\Delta x = a$很小时，Δp很大，使ΔE也很大，以至可以有：$\Delta E > E_{p0} - E \rightarrow E + \Delta E > E_{p0}$

经典



隧道效应

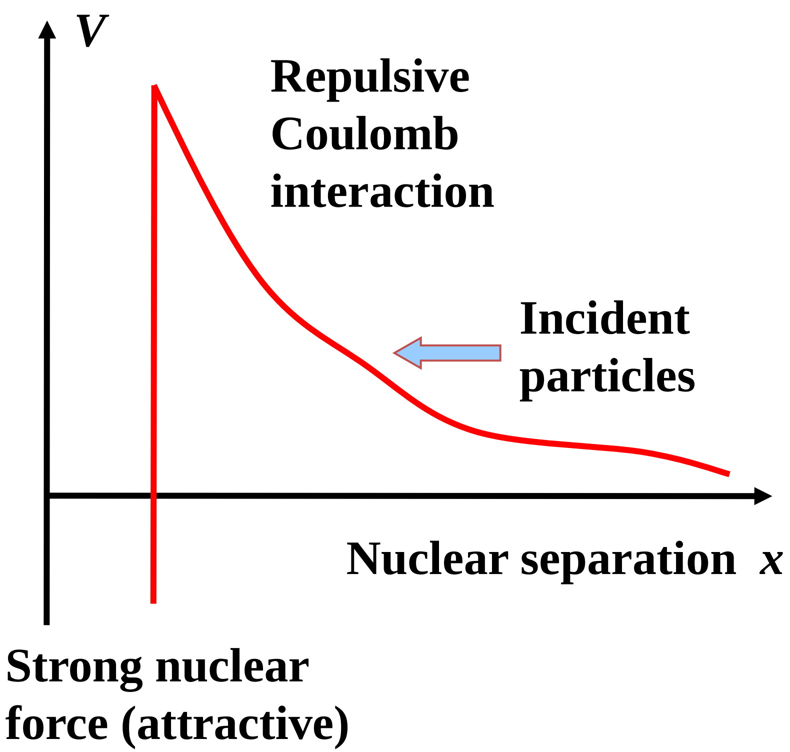
量子



崂山道士穿墙而过

隧道效应应用举例

(1) 核聚变



势垒高度 $\dfrac{(Ze)^2}{4\pi\varepsilon_0 r_{\text{nucleus}}}$ **~MeV**

热能(T =10^7 K)~keV

设动能按 Boltzmann分布,

$$P(E)\propto e^{-E/kT}$$

具有MeV能量核子的概率为 e^{-1000}

核子通过隧道效应穿透库仑势垒进入.

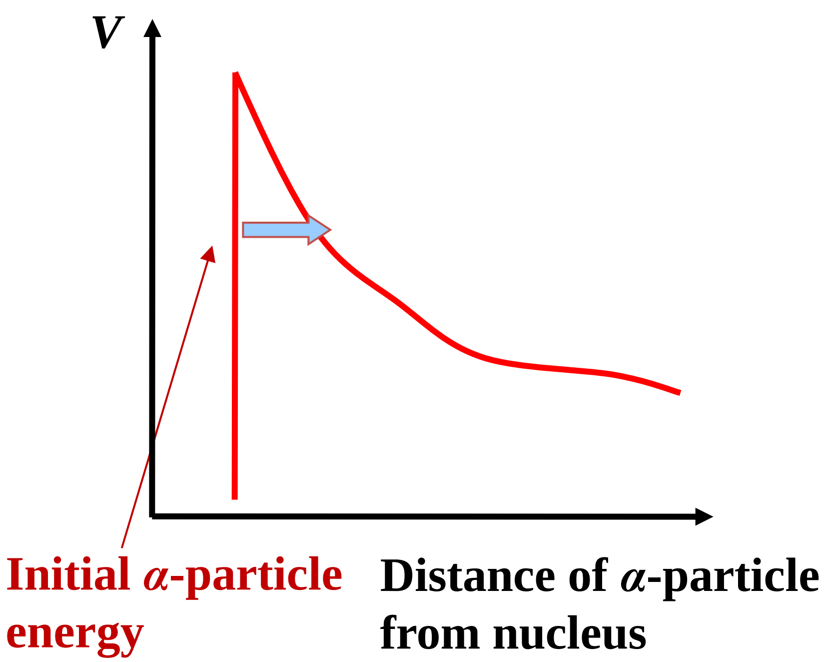
(2) 放射性α衰变

α粒子从放射性核中逸出—衰变.

^{238}U核:

库仑势垒V_0 = 35 MeV

α粒子能量E_α= 4.2 MeV

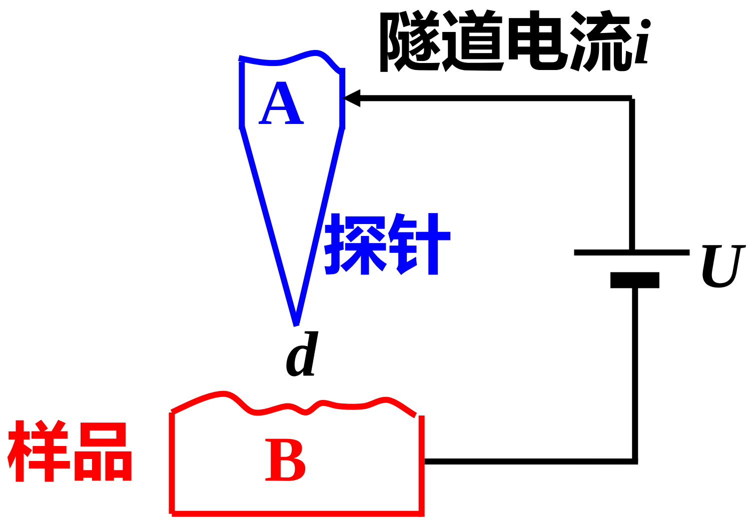


理论计算表明:

α粒子通过隧道效应穿透库仑势垒而跑出.

(3) 扫描隧道显微镜

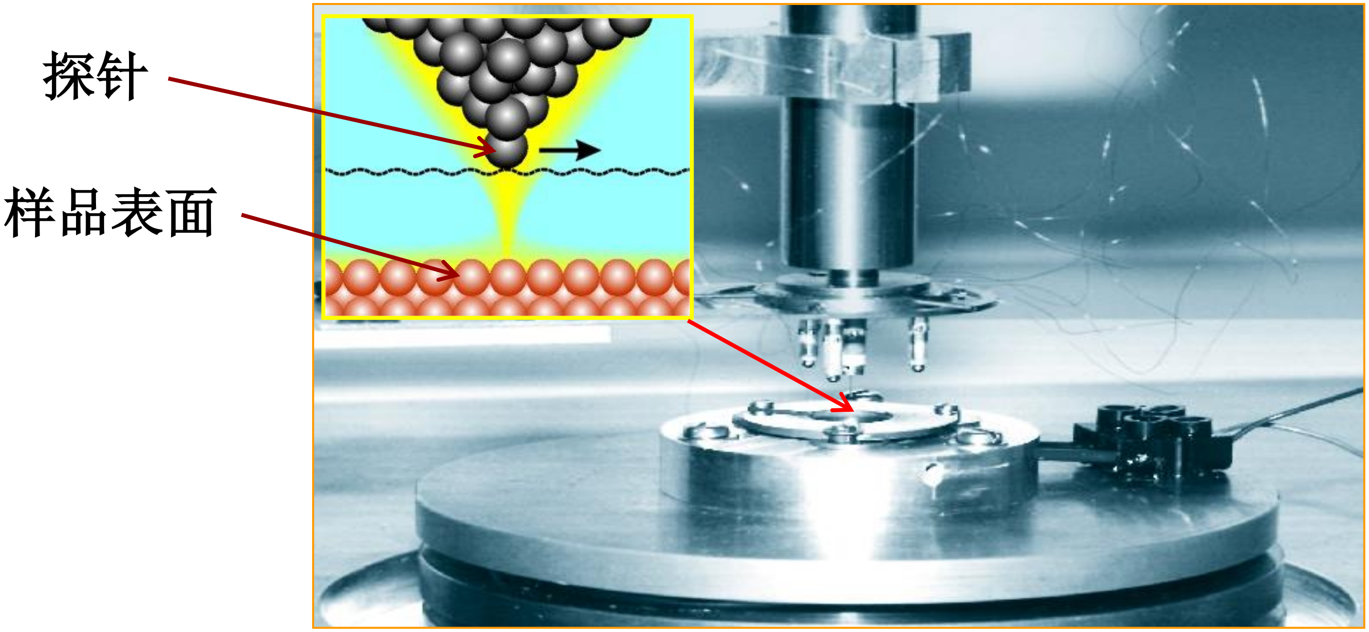
1981年宾尼希(G. Binig)和罗雷尔(H. Rohrer)利用电子的隧道效应制成 了扫描隧道显微镜（STM），可观测固体表面原子排列的状况．1986年宾尼希又研制了原子力显微镜.

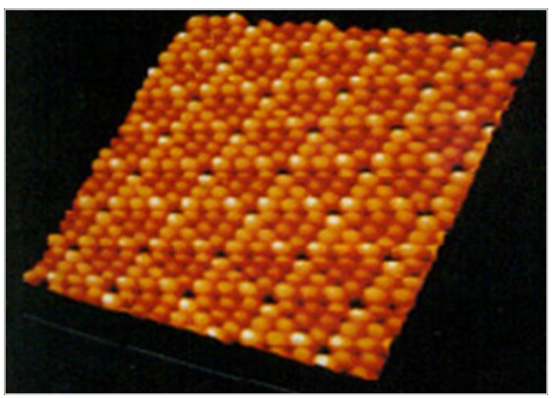


原理：利用量子力学的隧道效应

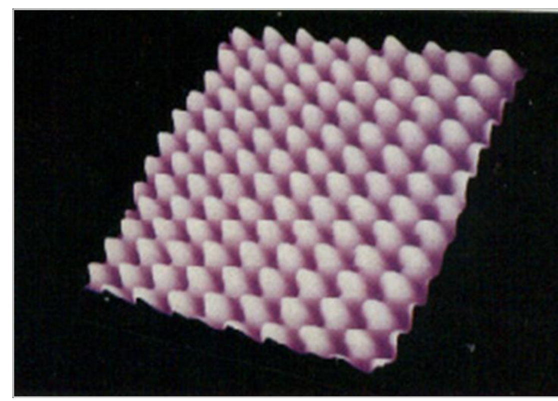
分辨率：横向 **0.1 nm**，纵向 **0.001 nm**

可以分辨出表面单个原子和原子台阶，原子结构，超晶格结构，表面缺陷细节，观测活体 DNA 基因、病毒。

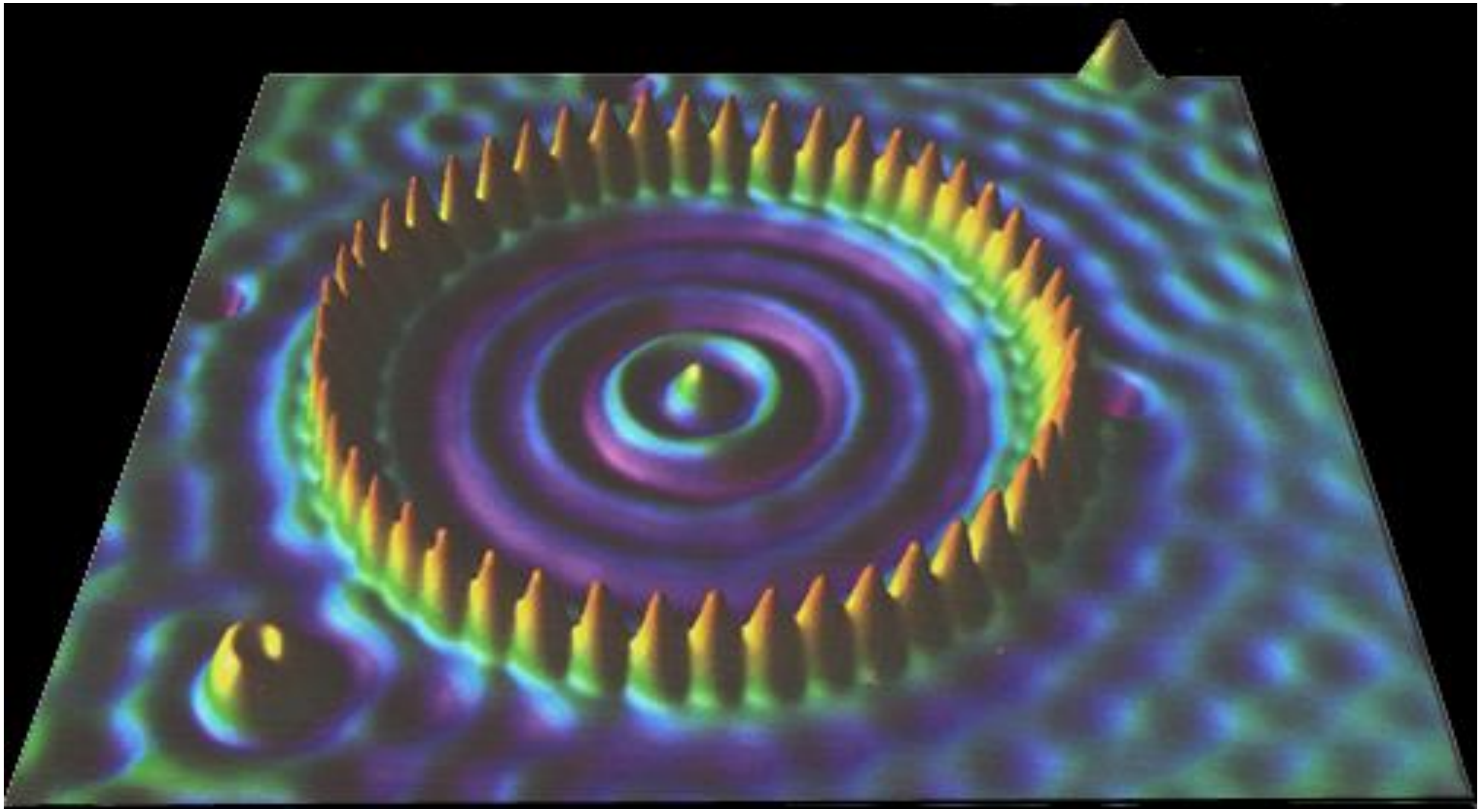




硅表面硅原子的排列



砷化镓表面砷原子的排列



1993年美国加州 IBM Almaden 研究中心的研究人员，用扫描隧穿显微镜(STM)操纵，将48个铁原子在铜的表面排列成一个圆圈，形成量子围栏(Quantum Corral)，电子被束缚在其中，其波函数形成同心圆状涟漪细浪。

五 一维线性谐振子 宇称 (Parity)

1. 势函数 $V(x)=\frac{1}{2}kx^2=\frac{1}{2}m\omega^2x^2$

m **— 振子质量,** $\boldsymbol{\omega}$ **— 固有频率,** ***x*** **— 位移.**

2. 定态薛定谔方程

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{2}m\omega^2x^2\right]\psi(x)=E\psi(x)$$

(1) 能量本征值

$$E_n=(n+\frac{1}{2})\hbar\omega=(n+\frac{1}{2})h\nu \quad (n=0,1,2,\cdots)$$

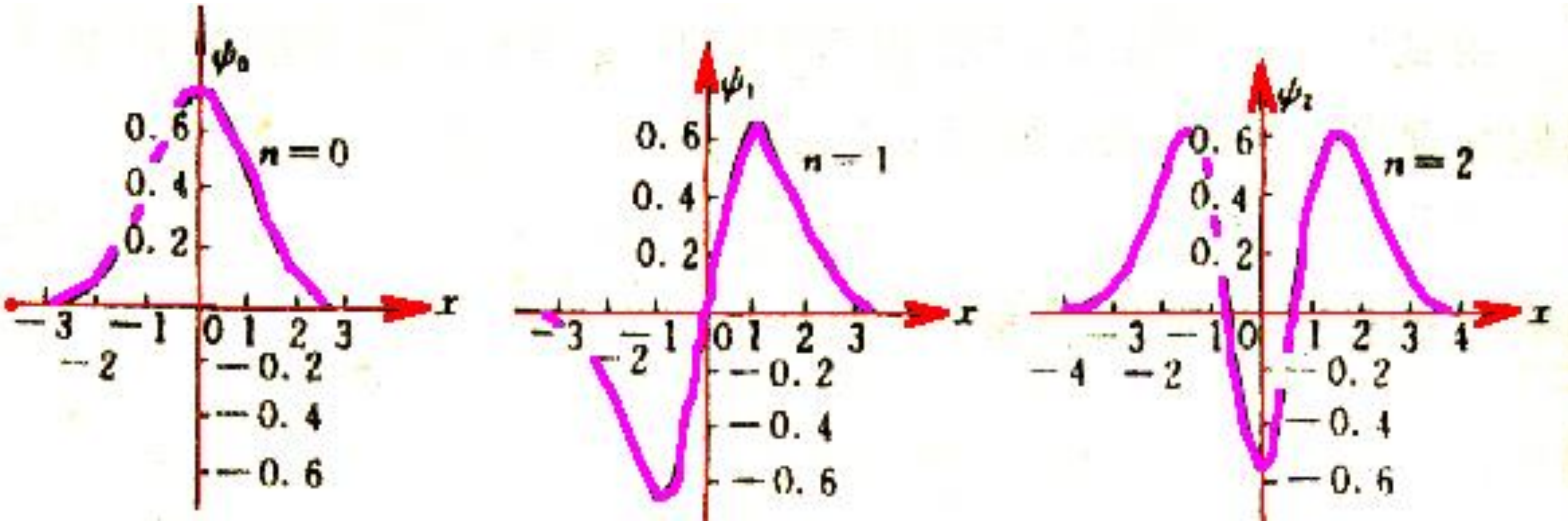
(2) 定态波函数（*参考*）

$$\psi_n(x)=A_n e^{-\alpha^2x^2/2}H_n(\alpha x)$$

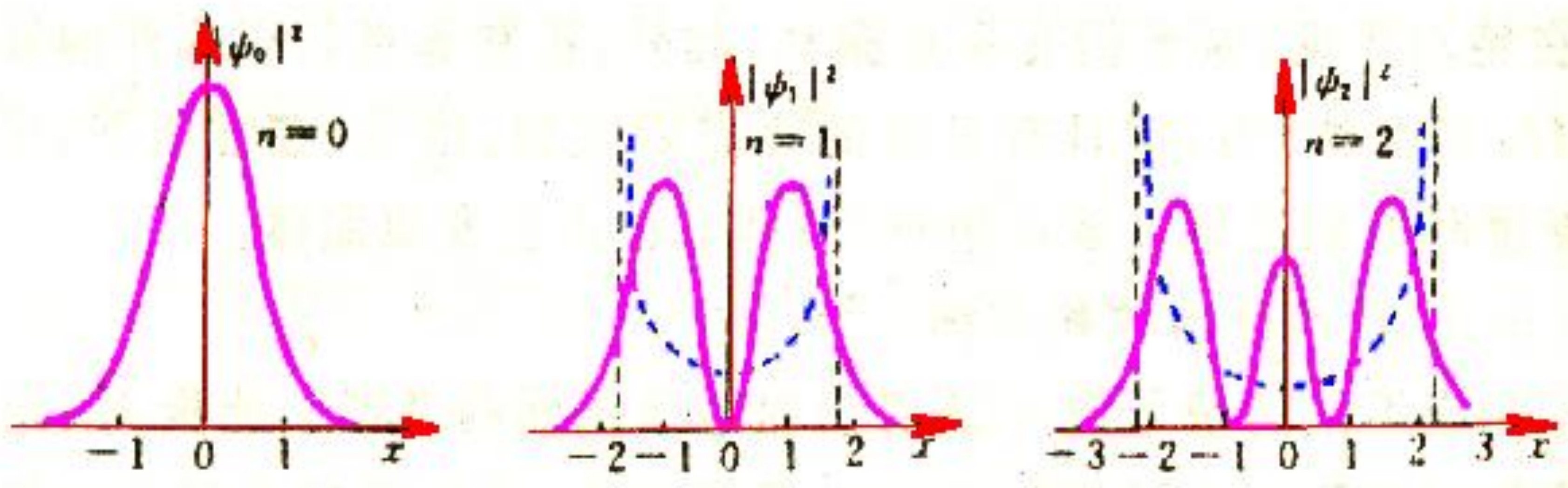
$$A_n=\sqrt{\frac{\alpha}{2^n n!\sqrt{\pi}}} \qquad \alpha=\sqrt{\frac{m\omega}{\hbar}}$$

$H_n(\alpha x)$:厄米多项式

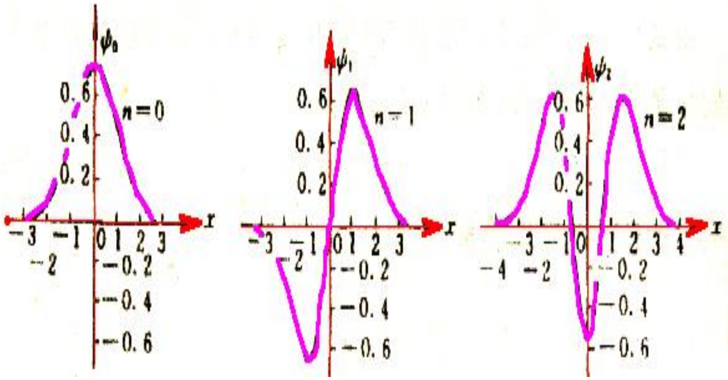
$$\psi_n(x) = A_n e^{-\alpha^2 x^2/2} H_n(\alpha x)$$

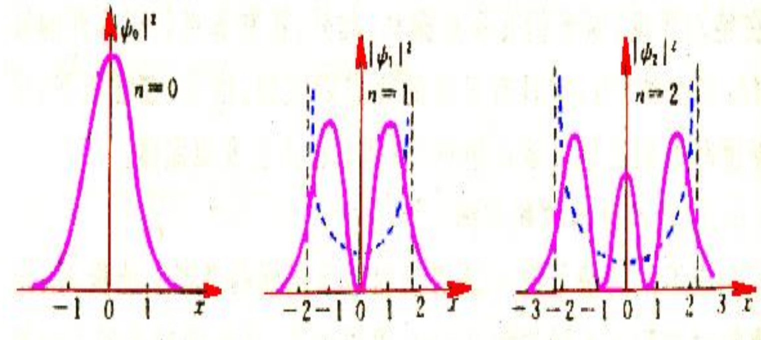


线性谐振子的波函数



线性谐振子的位置概率密度分布





讨论:

1.由图可见

当为 n偶数时: $\psi_n(-x)=\psi_n(x)$ 线性谐振子处于偶宇称

当为 n奇数时: $\psi_n(-x)=-\psi_n(x)$ 线性谐振子处于奇宇称

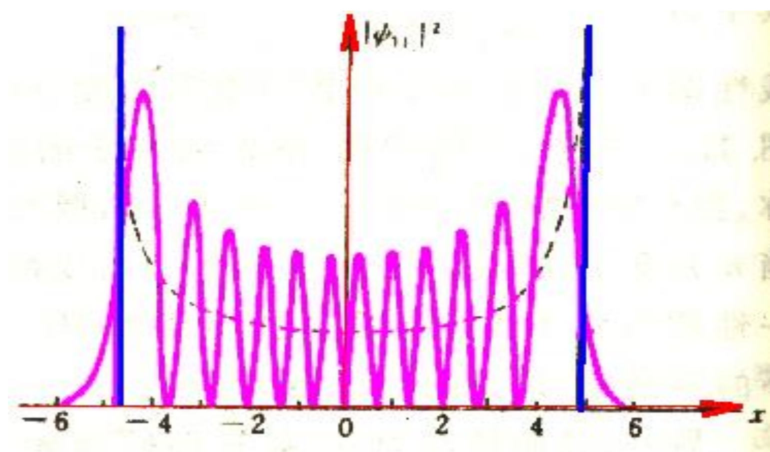
来源于 $x\rightarrow -x, U(-x)=U(x)$ 空间反演（宇称）不变性

2. 量子力学n较小时, 位置的概率密度分布与经典完全不同;

量子: 在 $x=0$处几率最大.

经典: 在 $x=0$处几率最小.

随着 n↑, 如n=11时量子和经典在平均上比较符合.



一维谐振子能级和概率密度分布

$$\therefore E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

能量特点:

(1) 量子化 等间距

$$\Delta E = h\nu$$

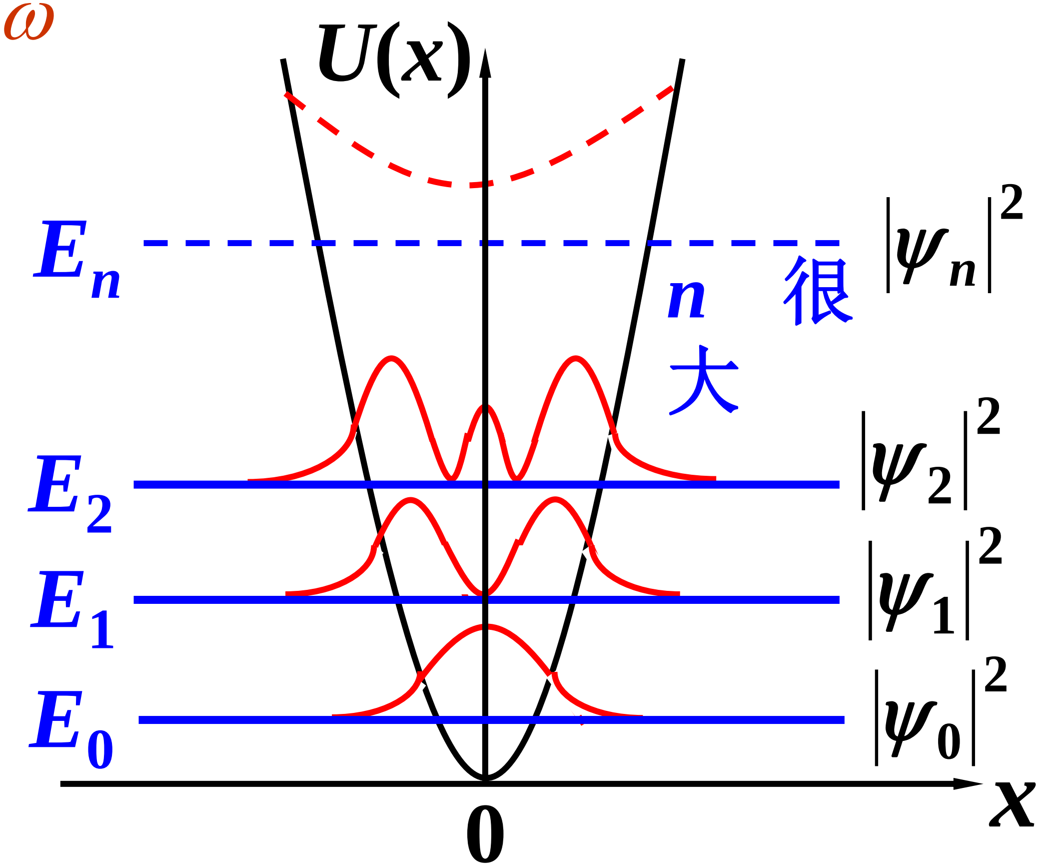
(2) 有零点能 $E_0 = \dfrac{1}{2}h\nu$

符合对应原理

当 $n \to \infty$

$$\frac{\Delta E}{E} \Rightarrow 0$$

能量可以连续变化（经典）



概率分布特点:

$E < U$ 区有隧道效应

宇称

对于本征波函数 $\psi_n(x)$，

$$\psi_n(-x) = (-1)^n \psi_n(x)$$

n 的奇偶性决定了本征函数的奇偶性.

一般，把由偶函数描述的量子态称为偶宇称态 **(Even parity state)**; 把由奇函数描述的量子态称为奇宇称态**(Odd parity state)** .

对于一维束缚定态，如果势能函数是对称的，则本征函数具有确定的宇称（**+1** 或 **-1**）.

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Question of Parity Conservation in Weak Interactions*

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AND

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(Received June 22, 1956)

The question of parity conservation in β decays and in hyperon and meson decays is examined. Possible experiments are suggested which might test parity conservation in these interactions.

RECENT experimental data indicate closely identical masses[1] and lifetimes[2] of the $\theta^+(\equiv K_{\pi 2}{}^+)$ and the $\tau^+(\equiv K_{\pi 3}{}^+)$ mesons. On the other hand, analyses[3] of the decay products of τ^+ strongly suggest on the grounds of angular momentum and parity conservation that the τ^+ and θ^+ are not the same particle. This poses a rather puzzling situation that has been extensively discussed.[4]

One way out of the difficulty is to assume that parity is not strictly conserved, so that θ^+ and τ^+ are two different decay modes of the same particle, which necessarily has a single mass value and a single lifetime. We wish to analyze this possibility in the present paper against the background of the existing experimental evidence of parity conservation. It will become clear that existing experiments do indicate parity conservation in strong and electromagnetic interactions to a high degree of accuracy, but that for the weak interactions (i.e., decay interactions for the mesons and hyperons, and various Fermi interactions) parity conservation is so far only an extrapolated hypothesis unsupported by experimental evidence. (One might even say that the present $\theta-\tau$ puzzle may be taken as an indication that parity conservation is violated in weak interactions. This argument is, however, not to be taken seriously because of the paucity of our present knowledge concerning the nature of the strange particles. It supplies rather an incentive for an examination of the question of parity conservation.) To decide unequivocally whether parity is conserved in weak interactions, one must perform an experiment to determine whether weak interactions differentiate the right from the left. Some such possible experiments will be discussed.

PRESENT EXPERIMENTAL LIMIT ON PARITY NONCONSERVATION

If parity is not strictly conserved, all atomic and nuclear states become mixtures consisting mainly of the state they are usually assigned, together with small percentages of states possessing the opposite parity. The fractional weight of the latter will be called $\mathfrak{F}^2$. It is a quantity that characterizes the degree of violation of parity con

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*参考：量子力学中的一些基本原理与数学表达

一、算符的定义

作用在一个函数上得到另一函数的运算(变换)符号

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

例如 $\quad \hat{F} = \dfrac{\mathrm{d}}{\mathrm{d}x} \qquad \hat{F} = \sqrt{} \qquad \hat{F} = (\quad)^*$

算符只是一种运算符号，它单独存在是没有意义的。它作用于波函数上，实现相应的运算才有意义。

$$\hat{A}\hat{B}\psi = \hat{A}(\hat{B}\psi)$$

一般 $\quad \hat{A}\hat{B} \neq \hat{B}\hat{A}$

二、算符的本征（特征）值方程

对于算符 $\hat{F}$，如果

$$\hat{F}\varphi_n(\vec{r}) = \lambda_n\varphi_n(\vec{r}) \qquad \lambda_n \text{ 为常数}$$

则称λ_n为$\hat{F}$的本征值。$\varphi_n(\vec{r})$为与λ_n相应的本征函数。

若与本征值λ_n相应的线性无关的本征函数共m个，则称为m度简并；若$m=1$，则称为非简并。

厄米算符

一个算符$\hat{O}$，如果对任意函数φ和ψ均满足

$$\int \psi^* \hat{O}\phi \cdot \mathrm{d}\tau = \int (\hat{O}\psi)^* \phi \cdot \mathrm{d}\tau$$

则称该算符为厄米算符

厄米算符的本征值为实数，属于不同本征值的本征函数是正交的。

三、力学量的算符表示

量子力学中，力学量用一个线性厄米算符表示，物理量的可能取值是相应算符的本征值。

在坐标空间中，有经典对应的力学量

$$F = F(\vec{r}, \vec{p}, t) \quad \Rightarrow \hat{F} = \hat{F}(\hat{\vec{r}}, \hat{\vec{p}}, t) = \hat{F}(\vec{r}, -\mathrm{i}\hbar\nabla, t)$$

坐标算符 $\hat{\vec{r}} = \vec{r}$

动量算符 $\boxed{\hat{\vec{p}} = -\mathrm{i}\hbar\nabla}$

动能算符 $\boxed{\hat{T} = \dfrac{\hat{\vec{p}}^2}{2m} = -\dfrac{\hbar^2}{2m}\nabla^2} = -\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}\right)$

力学量的平均值

$$\boxed{\overline{F} = \langle F \rangle = \iiint \psi^* \hat{F} \psi \mathrm{d}\vec{r}}$$

薛定谔方程

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}=[-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})]\psi(\vec{r},t)$$

$$-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r},t) \Rightarrow \frac{\hat{\vec{p}}^2}{2m}+U(\vec{r})$$

$$\Rightarrow \frac{\vec{p}^2}{2m}+U(\vec{r})=H$$

$$\hat{H}=\hat{H}(\vec{r},\hat{\vec{p}})=-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})$$ 哈密顿算符

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}=\hat{H}\psi(\vec{r},t)$$

定态薛定谔方程

$$\hat{H}\psi(\vec{r},t)=E\psi(\vec{r},t)$$

哈密顿算符的本征值方程

例：粒子在一维无限深势井中运动,其波函数为

$$\begin{cases}\psi_n(x)=\sqrt{\dfrac{2}{a}}\sin\left(\dfrac{n\pi x}{a}\right) & (0<x<a)\\ 0 & (x\le 0\text{或}x\ge a)\end{cases}$$

计算动量和动能的平均值。

解：动量算符为 $\hat{p}_x=-i\hbar\dfrac{\partial}{\partial x}$

动量的平均值为:

$$\bar{p}_x=\int\psi_{\mathrm{n}}^*(x)\,\hat{p}_x\psi_{\mathrm{n}}(x)\,\mathrm{d}x=\int\psi_{\mathrm{n}}^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_{\mathrm{n}}(x)\,\mathrm{d}x$$

$$=-i\frac{2\hbar}{a}\int_0^a\sin\left(\frac{n\pi x}{a}\right)\frac{\partial}{\partial x}\sin\left(\frac{n\pi x}{a}\right)\mathrm{d}x$$

$$=-i\frac{2\hbar}{a}\left(\frac{n\pi}{a}\right)\int_0^a\sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right)\mathrm{d}x=0$$

动能算符为 $\hat{T}=\frac{\hat{p}_x^2}{2m}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

动能的平均值为

$$\bar{T}=\int\psi_{\mathrm{n}}^*(x)\hat{T}\psi_{\mathrm{n}}(x)\,\mathrm{d}x=\int\psi_{\mathrm{n}}^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi_{\mathrm{n}}(x)\,\mathrm{d}x$$

$$=-\frac{\hbar^2}{ma}\int_0^a\sin\left(\frac{n\pi x}{a}\right)\frac{\partial^2}{\partial x^2}\sin\left(\frac{n\pi x}{a}\right)\mathrm{d}x$$

$$=\frac{\hbar^2}{ma}\left(\frac{n\pi}{a}\right)^2\int_0^a\sin\left(\frac{n\pi x}{a}\right)^2\mathrm{d}x=\frac{\hbar^2n^2\pi^2}{2ma^2}$$

量子力学的基本原理

量子力学中，微观系统的力学量要用一个线性厄米算符表示。在坐标空间中，对有经典对应的力学量

$$F = F(\vec{r}, \vec{p}, t)$$

$$\hat{F} = \hat{F}(\hat{\vec{r}}, \hat{\vec{p}}, t) = \hat{F}(\vec{r}, -\mathrm{i}\hbar\nabla, t)$$

物理量的可能取值是相应算符的本征值。

$$\hat{F}\varphi_i = a_i\varphi_i$$

若系统处于态矢量ψ所描写的状态，

$$\psi = \sum_i c_i\varphi_i \quad \text{而} \quad c_i = \int \varphi_i^* \psi \, \mathrm{d}\tau$$

在ψ状态下，测量物理量F得到结果a_i的概率为

$$P_i = |c_i|^2$$

五、对易关系

经典力学量 $xp_x = p_x x$ 交换律，可对易

量子力学 $\hat{x} = x$ $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

$$\hat{x}\hat{p}_x \overset{?}{=} \hat{p}_x\hat{x}$$

$$(\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi = (-i\hbar x\frac{\partial}{\partial x} + i\hbar\frac{\partial}{\partial x}x)\psi$$

$$= -i\hbar x\frac{\partial \psi}{\partial x} + i\hbar\psi + i\hbar x\frac{\partial \psi}{\partial x} = i\hbar\psi$$

$(\hat{x}\hat{p}_x - \hat{p}_x\hat{x}) = i\hbar \neq 0$ 不对易，***x*, *p***的值不能同时确定

记 $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ 算符 $\hat{A}$ 和 $\hat{B}$ 的对易关系

若 $[\hat{A}, \hat{B}] = 0$ 算符 $\hat{A}$ 和 $\hat{B}$ 是对易的

六、常用算符

动量算符 $$\hat{\vec{p}} = -i\hbar[\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}] = -i\hbar\nabla$$

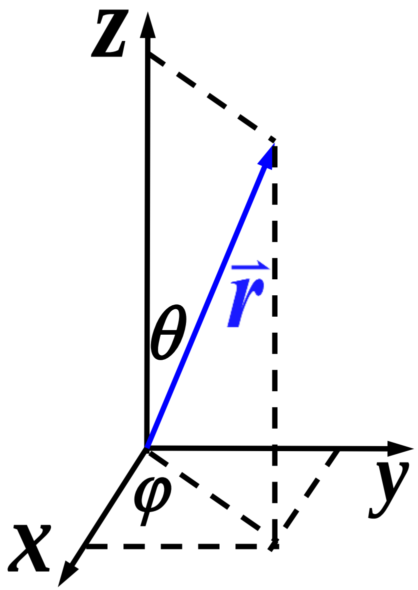
动能算符 $$\hat{T} = \frac{\hat{\vec{p}}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$$

哈密顿算符(能量算符) $$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + U(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$$

角动量算符

$$\hat{\vec{L}} = \vec{r}\times\hat{\vec{p}} = -i\hbar\vec{r}\times\nabla = -i\hbar\begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix} \Rightarrow \begin{cases} \hat{L}_x = -i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}) \\ \hat{L}_y = -i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}) \\ \hat{L}_z = -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \end{cases}$$

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



$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

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

$$x = r\sin\theta\cdot\cos\varphi$$

$$y = r\sin\theta\cdot\sin\varphi$$

$$z = r\cos\theta$$

$$\hat{L}_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + ctg\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + ctg\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \arctan\left[\frac{\sqrt{x^2 + y^2}}{z}\right]$$

$$\varphi = \arctan\left[\frac{y}{x}\right]$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$$

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right]$$

$$\begin{aligned}
\nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\
&= \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \\
&= \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{r^2\hbar^2} \hat{L}^2
\end{aligned}$$

*转化过程（参考）：

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

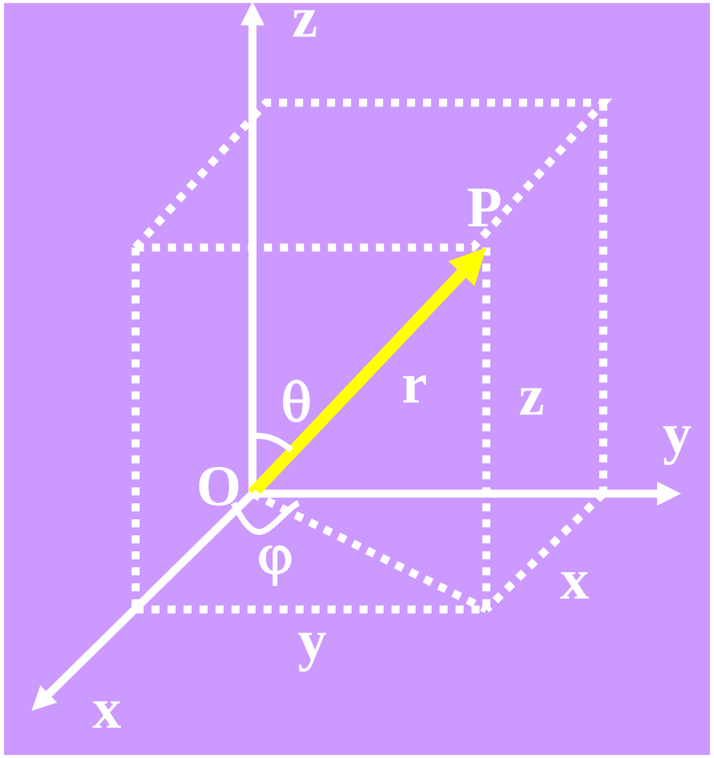
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2\hbar^2}\hat{L}^2$$

$$r = \sqrt{x^2 + y^2 + z^2} \qquad x = r\sin\theta\cos\varphi$$

$$\theta = \arccos\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right) \qquad y = r\sin\theta\sin\varphi$$

$$\varphi = arctg\left(\frac{y}{x}\right) \qquad z = r\cos\theta$$



$$x = r\sin\theta\cos\varphi \qquad r^2 = x^2 + y^2 + z^2$$

$$y = r\sin\theta\sin\varphi \qquad \cos\theta = \frac{z}{r} \qquad tg\varphi = \frac{y}{x}$$ 两边对x求偏导

$$z = r\cos\theta$$

两边对x求偏导

$$\frac{\partial\theta}{\partial x} = \frac{1}{\sin\theta}\frac{z}{r^2}\frac{\partial r}{\partial x} = \frac{1}{r}\cos\theta\cos\varphi$$

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin\theta\cos\varphi$$

$$\frac{\partial\varphi}{\partial x} = -\frac{1}{\sec^2\varphi}\frac{y}{x^2} = -\frac{\sin\varphi}{r\sin\theta}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{1}{r}\frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial y}\frac{\partial}{\partial\varphi} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{1}{r}\frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial z}\frac{\partial}{\partial\varphi} = \cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}$$

$$\frac{\partial}{\partial x}=\frac{\partial r}{\partial x}\frac{\partial}{\partial r}+\frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta}+\frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}=\sin\theta\cos\varphi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta}-\frac{1}{r}\frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial y}=\frac{\partial r}{\partial y}\frac{\partial}{\partial r}+\frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta}+\frac{\partial\varphi}{\partial y}\frac{\partial}{\partial\varphi}=\sin\theta\sin\varphi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta}+\frac{1}{r}\frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial z}=\frac{\partial r}{\partial z}\frac{\partial}{\partial r}+\frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta}+\frac{\partial\varphi}{\partial z}\frac{\partial}{\partial\varphi}=\cos\theta\frac{\partial}{\partial r}-\frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}$$

$$\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\frac{\partial}{\partial x}\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\frac{\partial}{\partial y}+\frac{\partial}{\partial z}\frac{\partial}{\partial z}$$

$$=(\sin\theta\cos\varphi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta}-\frac{1}{r}\frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi})\ (\sin\theta\cos\varphi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta}-\frac{1}{r}\frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi})$$

$$+(\sin\theta\sin\varphi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta}+\frac{1}{r}\frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi})(\sin\theta\sin\varphi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta}+\frac{1}{r}\frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi})$$

$$+(\cos\theta\frac{\partial}{\partial r}-\frac{1}{r}\sin\theta\frac{\partial}{\partial\theta})\ (\cos\theta\frac{\partial}{\partial r}-\frac{1}{r}\sin\theta\frac{\partial}{\partial\theta})$$

$$=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})+\frac{1}{r^2(\sin\theta)^2}\frac{\partial^2}{\partial\varphi^2}$$

§ 9　氢原子的量子理论

氢原子中电子的势能函数

$$E_{\mathrm{p}} = -\frac{e^2}{4\pi\varepsilon_0 r}$$

定态薛定谔方程为

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)\psi = 0$$

转化为球坐标

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$

$$+\frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)\psi = 0$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r})+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\frac{\partial\psi}{\partial\theta})+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$
$$+\frac{8\pi^2 m}{h^2}(E+\frac{e^2}{4\pi\varepsilon_0 r})\psi=0$$

分离变量法求解, 设

$$\psi(r,\theta,\varphi)=R(r)\Theta(\theta)\Phi(\varphi)$$

得
$$\begin{cases}\dfrac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}+m_l{}^2\Phi=0\\[2ex]\dfrac{m_l{}^2}{\sin^2\theta}-\dfrac{1}{\Theta\sin\theta}\dfrac{\mathrm{d}}{\mathrm{d}\theta}(\sin\theta\dfrac{\mathrm{d}\Theta}{\mathrm{d}\theta})=l(l+1)\\[2ex]\dfrac{1}{R}\dfrac{\mathrm{d}}{\mathrm{d}r}(r^2\dfrac{\mathrm{d}R}{\mathrm{d}r})+\dfrac{8\pi^2 mr^2}{h^2}(E+\dfrac{e^2}{4\pi\varepsilon_0 r})=l(l+1)\end{cases}$$