第 4 章 薛定锷方程与定态波函数

与t无关！

4.1. 一维定态问题

4.2. 谐振子

4.1 一维定态问题

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)\right)\psi(x,t)$$

令 $\psi(x,t)=\psi(x)f(t)$ 对时间求导 $\rightarrow\dfrac{\partial\psi(x,t)}{\partial t}=\psi(x)\dfrac{\partial f(t)}{\partial t}$

对空间二阶导数 $\rightarrow\dfrac{\partial^2\psi(x,t)}{\partial x^2}=f(t)\dfrac{\partial^2\psi(x)}{\partial x^2}$

将其代入薛定谔方程, 得

$$\rightarrow i\hbar\psi(x)\frac{\partial f(t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)\psi(x)f(t)$$ 移动同类 $$\rightarrow i\hbar\frac{\partial f(t)}{f(t)\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)$$

$$\rightarrow i\hbar\frac{\partial f(t)}{f(t)\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)=E$$

- 一个是变量为t 的方程

$$i\hbar\frac{\partial f(t)}{f(t)\partial t}=E \quad \text{积分} \rightarrow f = Ae^{-\frac{i}{\hbar}Et}$$

A是待定复常数， E有能量量纲,以后可知是粒子的能量：动能 + 势能）

- 一个是变量为x的方程

$$i\hbar\frac{\partial f(t)}{f(t)\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)=E \qquad \rightarrow\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)\psi(x)=E\psi(x)$$

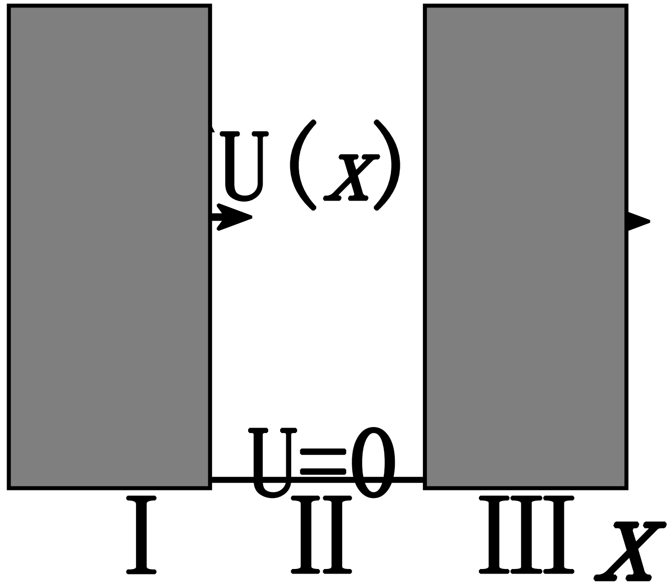
$$\rightarrow\hat{H}\psi(x)=E\psi(x)$$

其解ψ(x)与粒子所处的条件外力场有关。 $|\psi(x,t)|^2 \propto \left|\psi(x)e^{-\frac{i}{\hbar}\mathrm{E}t}\right|^2=|\psi(x)|^2$

即定态时，概率密度可以用$|(x)|^2$来表示，(x)称为<u>定态波函数</u>，

1. 无限深方势阱中的粒子

金属中自由电子的运动，是被限制在一个有限的范围称为束缚态。作为粗略的近似，我们认为这些电子在一维无限深方势阱中运动：



无限深方势阱

它的势能函数为

$$U(x)=\begin{cases}0, & 0\le x\le a\\ \infty, & |x|>a\end{cases}$$

按照一维定态薛谔定方程

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)\psi(x)=E\psi(x)$$

由于在I、III两区的U(x)＝∞，显然应$\psi_I=0$；$\psi_{III}=0$，否则方程就无意义了。

由于II区的 U(x)= 0，因此该区薛定谔方程为

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)\psi(x)=E\psi(x)$$

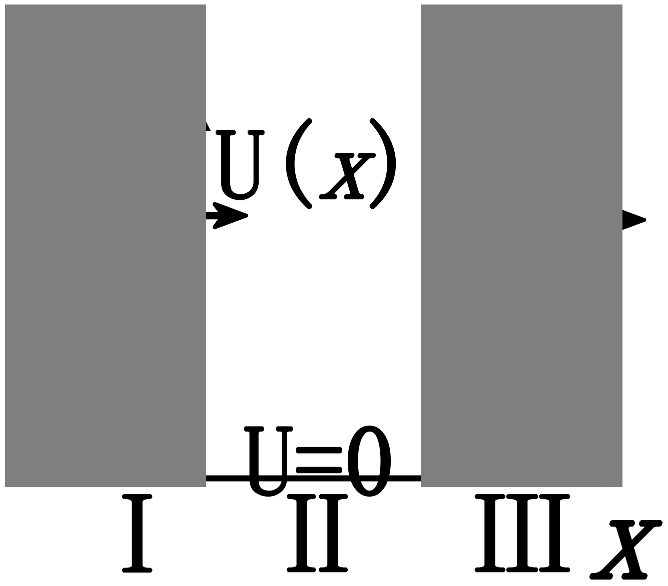
$$U=0\rightarrow-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}=E\psi(x)$$

令 $\rightarrow k^2=\frac{2m}{\hbar^2}E \quad \rightarrow\frac{\partial^2\psi(x)}{\partial x^2}=-k^2\psi(x)$

$$\rightarrow\psi(x)=A\sin(kx+\theta)$$

$\psi(x)$在$x=0$和$x=a$处必须连续

$$\rightarrow\begin{cases}A\sin(\theta)=0,\\A\sin(ka+\theta)=0,\end{cases}\rightarrow\rightarrow\begin{cases}\theta=0\\ka=n\pi\end{cases}\rightarrow\psi_o=A\sin\frac{n\pi}{a}x$$



无限深方势阱

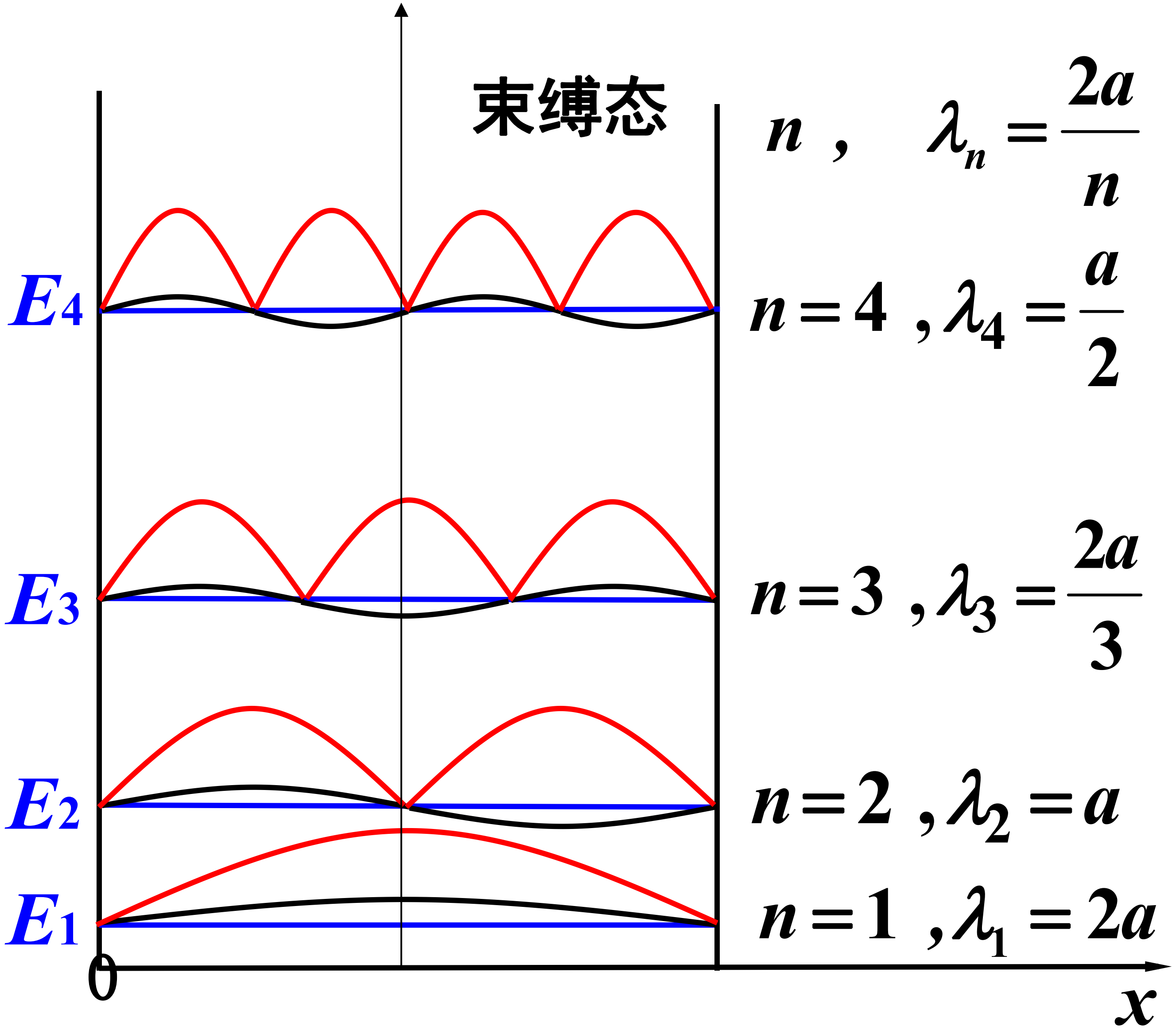
归一化条件 $\rightarrow \int_0^{2a} (\psi_o)^2 dx = \int_0^{2a} \left(A\sin\frac{n\pi}{a}x \right)^2 = 1 \qquad A = \sqrt{\frac{2}{a}}$

$$\rightarrow \begin{cases} \psi_o = A\sin\frac{n\pi}{a}x & 0 \le x \le a \\ \psi_o = 0 & x \ge a, x \le 0 \end{cases}$$

$$令 \rightarrow k^2 = \frac{2m}{\hbar^2}E \rightarrow 代入得 \rightarrow \frac{2m}{\hbar^2}E = \frac{n^2\pi^2}{a^2} \rightarrow 得 E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

由每个能量本征波函数所描述的粒子的状态，是能量有确定值的状态称为粒子的能量本征态。

束缚态



$$n, \quad \lambda_n = \frac{2a}{n}$$

$$n = 4, \lambda_4 = \frac{a}{2}$$

$$n = 3, \lambda_3 = \frac{2a}{3}$$

$$n = 2, \lambda_2 = a$$

$$n = 1, \lambda_1 = 2a$$

例题1:在一维无限深势阱中运动的微观粒子，它的定态波函数如图a,对应的能量为4eV。如它的一个波函数为b,它的总能量为多少?粒子的零点能为多少?

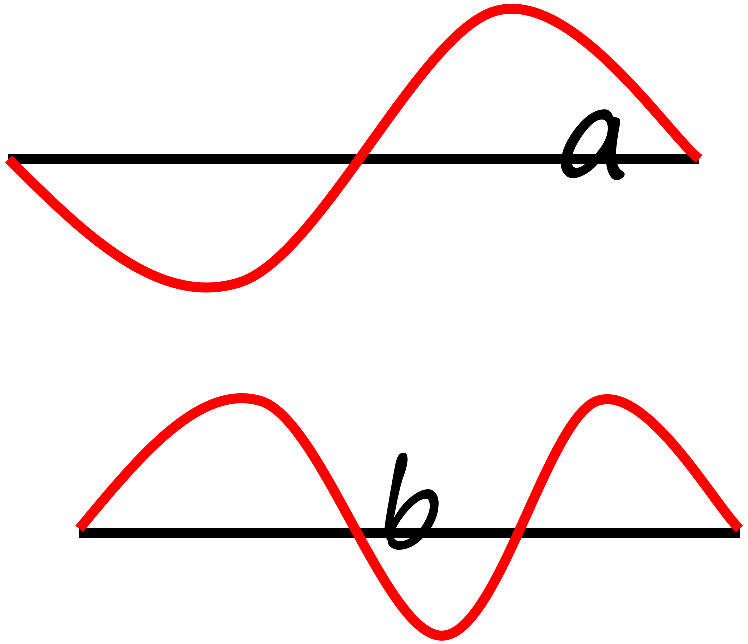
解:

$$E = n^2 \frac{\pi^2\hbar^2}{2ma^2} = n^2 E_0,$$

$$4 = 2^2 \frac{\pi^2\hbar^2}{2ma^2} = 4E_0$$

$$E = n^2 \frac{\pi^2\hbar^2}{2ma^2}$$

$$E_3 = 3^2 E_0 = 9$$



例题2：计算微观粒子出现概率最大的位置？

$$\psi\left(x,t\right)_n = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)e^{-\frac{a_n i}{\hbar}t} \qquad n = 1,2,3,4,5......$$

解：

$$F\left(x,t\right) = \psi^*\left(x,t\right)_n\psi\left(x,t\right)_n = \frac{2}{L}\cos^2\left(\frac{n\pi x}{L}\right)$$

$$\frac{\partial F\left(x,t\right)}{\partial x} = \frac{\partial}{\partial x}\left[\frac{2}{L}\cos^2\left(\frac{n\pi x}{L}\right)\quad\right] = \left|\frac{4}{L}\frac{n\pi}{L}\cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)\right| = 0$$

$$\left|\frac{4}{L}\frac{n\pi}{L}\cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)\right| = \left|\frac{2n\pi}{L^2}\sin\left(\frac{2n\pi x}{L}\right)\right| = 0$$

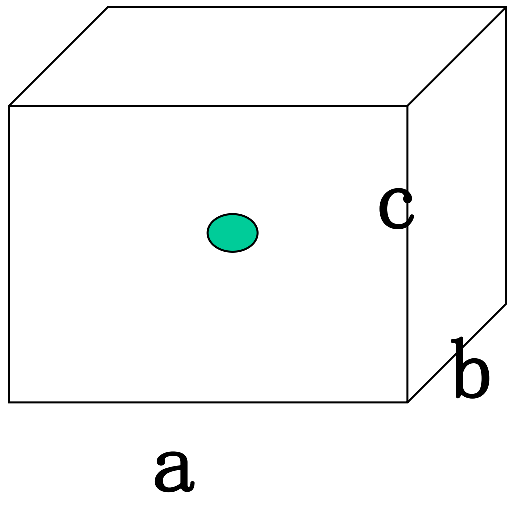
$$x = 0, \frac{L}{2}, L$$

2.三维无限深方势阱

三维无限深方势阱（考虑一个粒子被因禁在一个长方体盒子内，盒内U=0，盒外U=+∞，求能量本征值与本征函数）

解：
$$\left(-\frac{\hbar^2}{2m}\nabla^2+U(x,y,z)\right)\psi(x,y,z)=E\psi(x,y,z)$$

$$U=0\rightarrow\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(x,y,z)=E\psi(x,y,z)$$



存在 $\rightarrow\psi(x,y,z)=\psi(x)\psi(y)\psi(z)$

$$-\frac{\hbar^2}{2m}\left(\psi(y)\psi(z)\frac{\partial^2\psi(x)}{\partial x^2}+\psi(x)\psi(z)\frac{\partial^2\psi(y)}{\partial y^2}+\psi(x)\psi(y)\frac{\partial^2\psi(z)}{\partial z^2}\right)=E\psi(x)\psi(y)\psi(z)$$

$$\rightarrow-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x)}{\psi(x)\partial x^2}+\frac{\partial^2\psi(y)}{\psi(y)\partial y^2}+\frac{\partial^2\psi(z)}{\psi(z)\partial z^2}\right)=E$$

有：$k^2=\dfrac{2m}{\hbar^2}E$

$$有:k^2=\frac{2m}{\hbar^2}E\rightarrow k^2=k_x^2+k_y^2+k_z^2$$

$$\rightarrow\left(\frac{\partial^2\psi(x)}{\psi(x)\partial x^2}+\frac{\partial^2\psi(y)}{\psi(y)\partial y^2}+\frac{\partial^2\psi(z)}{\psi(z)\partial z^2}\right)=-k^2=-\left(k_x^2+k_y^2+k_z^2\right)$$

$$\rightarrow\begin{cases}\left(\dfrac{\partial^2\psi(x)}{\psi(x)\partial x^2}\right)=-k_x^2\\\left(\dfrac{\partial^2\psi(y)}{\psi(y)\partial y^2}\right)=-k_y^2\\\left(\dfrac{\partial^2\psi(z)}{\psi(z)\partial z^2}\right)=-k_z^2\end{cases}\quad 分别求解\rightarrow\begin{cases}\psi(x)=\sqrt{\dfrac{2}{a}}\sin\dfrac{n\pi}{a}x, & k_x=\dfrac{n\pi}{a}\\\psi(y)=\sqrt{\dfrac{2}{b}}\sin\dfrac{m\pi}{b}y & k_y=\dfrac{m\pi}{b}\\\psi(z)=\sqrt{\dfrac{2}{c}}\sin\dfrac{l\pi}{c}z & k_z=\dfrac{l\pi}{c}\end{cases}$$

$$\boldsymbol{\psi_{n,m,l}(x,y,z)=\psi(x)\psi(y)\psi(z)=\sqrt{\frac{8}{abc}}\sin\left(\frac{n\pi}{a}x\right)\sin\left(\frac{m\pi}{b}y\right)\sin\left(\frac{l\pi}{c}z\right)}$$

$$\text{利用}: k^2 = \frac{2m}{\hbar^2}E \rightarrow k^2 = k_x^2 + k_y^2 + k_z^2$$

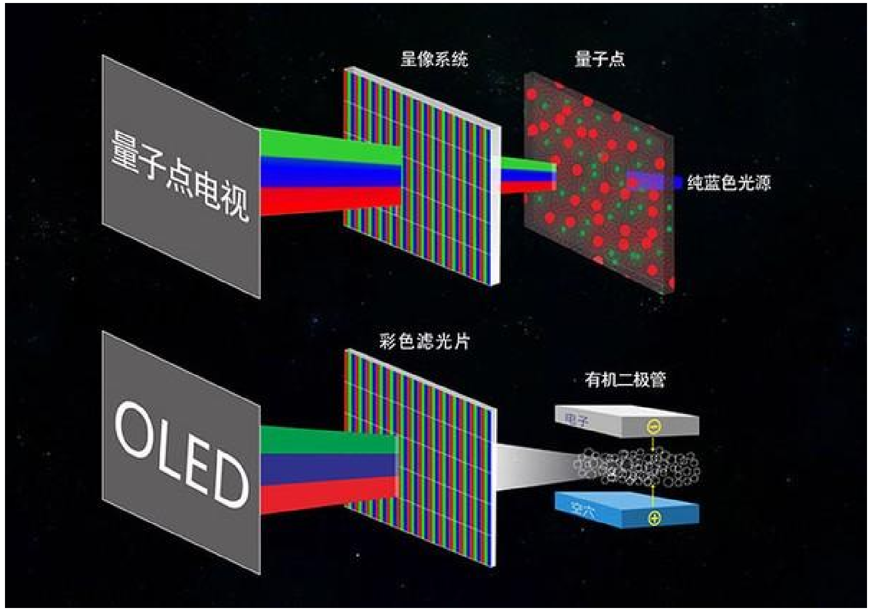
$$\text{利用} \rightarrow \begin{cases} \psi(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x, & k_x = \frac{n\pi}{a} \\ \psi(y) = \sqrt{\frac{2}{b}}\sin\frac{m\pi}{b}y & k_y = \frac{m\pi}{b} \\ \psi(z) = \sqrt{\frac{2}{c}}\sin\frac{l\pi}{c}z & k_z = \frac{l\pi}{c} \end{cases}$$

$$\boldsymbol{E_{\mathrm{n,m,l}} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \left(\frac{m\pi}{b}\right)^2 + \left(\frac{l\pi}{c}\right)^2\right] \qquad (n, l, m = 1, 2, 3, \ldots)}$$

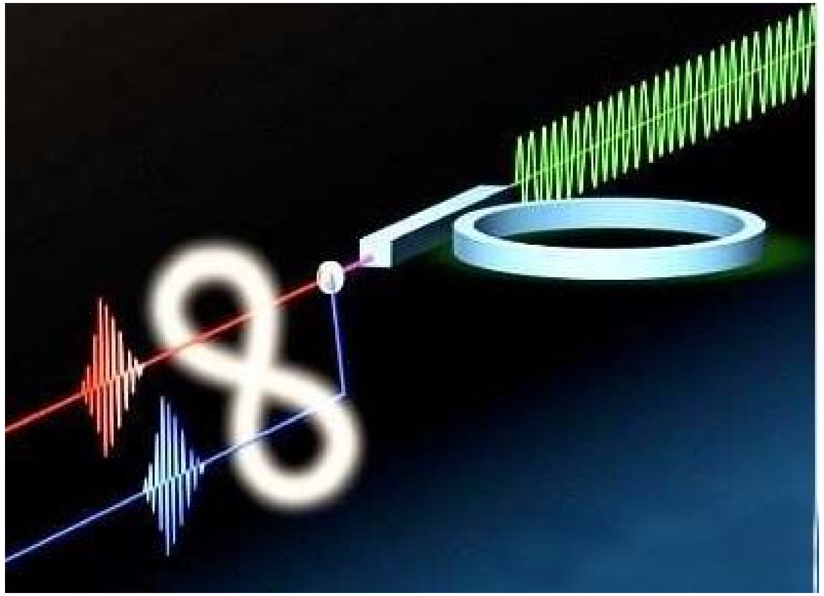
量子点的典型应用

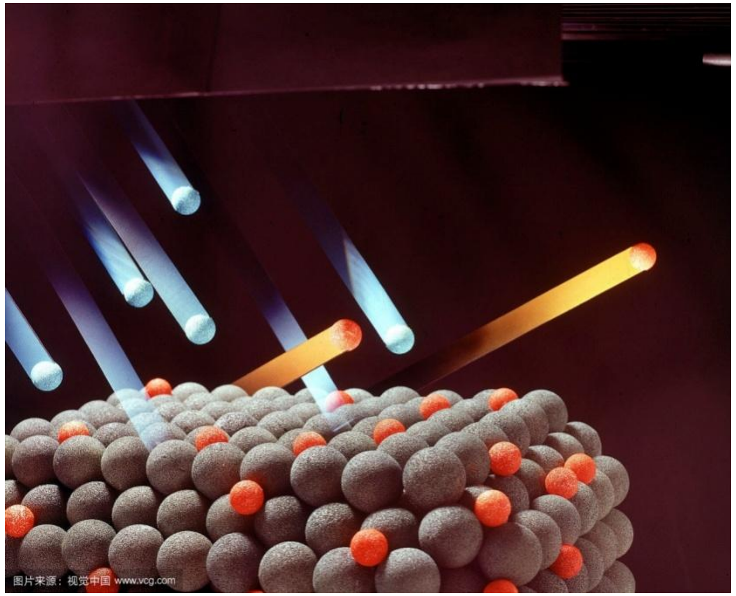
$$E_{\mathrm{n,m,l}}=\frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2)=\frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2+\left(\frac{m\pi}{b}\right)^2+\left(\frac{l\pi}{c}\right)^2\right]\qquad (n,l,m=1,2,3,\ldots)$$

量子点电视

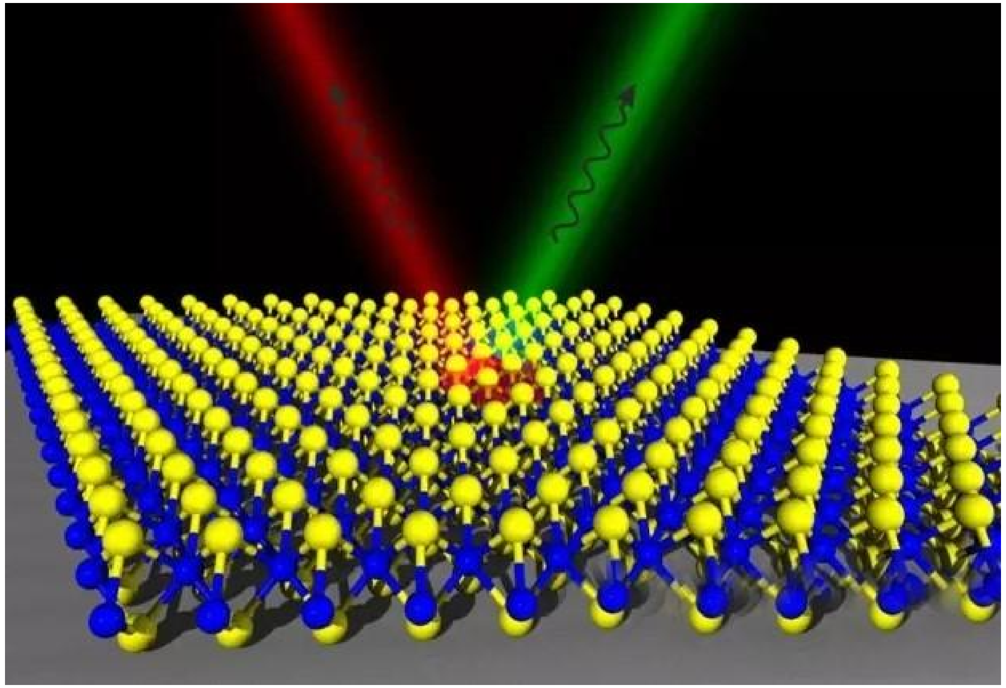


光子的分离





新型二维材料



3.一维有限深方势阱（一）

$$\left(-\frac{\hbar^2 d^2}{2mdx^2}+U\right)\psi(x)=E\psi(x)$$

$$\begin{cases}\dfrac{d^2\psi(x)}{dx^2}=-\dfrac{2m}{\hbar^2}E\psi(x) & -a\le x\le a\\ \dfrac{d^2\psi(x)}{dx^2}=-\dfrac{2m}{\hbar^2}(E-U)\psi(x) & x\le -a, x\ge a\end{cases}$$

$$\begin{cases}\alpha=\sqrt{\dfrac{2m_0}{\hbar^2}E}\\ \beta=\sqrt{\dfrac{2m_0}{\hbar^2}(U_0-E)}\end{cases}\rightarrow\begin{cases}\dfrac{d^2\psi(x)}{dx^2}=-\alpha^2\psi(x) & -a\le x\le a\\ \dfrac{d^2\psi(x)}{dx^2}=-\beta^2\psi(x) & x\le -a, x\ge a\end{cases}$$

$$一般解\rightarrow\begin{cases}\psi(x)=A_1e^{-i\beta x}+Ae^{i\beta x} & x<-a,\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x} & -a<x<a\\ \psi(x)=A_2e^{-i\beta x}+A'e^{i\beta x} & x>a\end{cases}$$

$$E<U_0,\beta=i\sqrt{\frac{2m_0}{\hbar^2}(U_0-E)}\to\begin{cases}\psi(x)=A_1e^{-ii\beta x}+A\ e^{ii\beta x}\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x}\\ \psi(x)=Ae^{-ii\beta x}+A_2e^{ii\beta x}\end{cases}\to\begin{cases}\psi(x)=A_1e^{\beta x} & x<-a,\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x} & -a<x<a\\ \psi(x)=A_2e^{-\beta x} & x>a\end{cases}$$

$$\text{对应的导数}\to\begin{cases}\psi'(x)=A_1\beta e^{\beta x} & x<-a,\\ \psi'(x)=i\alpha A_0e^{i\alpha x}-i\alpha B_0e^{-i\alpha x} & -a<x<a\\ \psi'(x)=-\beta A_2e^{-\beta x} & x>a\end{cases}$$

$$\begin{pmatrix}x=-a\\ x=a\end{pmatrix}\to\begin{cases}\psi(-a)=A_1e^{\beta a}\\ \psi(-a)=A_0e^{-i\alpha a}+B_0e^{i\alpha a}\\ \psi(a)=A_0e^{i\alpha a}+B_0e^{-i\alpha a}\\ \psi(a)=A_2e^{-\beta a}\end{cases}$$

$$\to\begin{cases}A_1e^{-\beta a}=A_0e^{-i\alpha a}+B_0e^{i\alpha a}=2A_0\cos\alpha a\\ A_2e^{-\beta a}=A_0e^{i\alpha a}+B_0e^{-i\alpha a}=2A_0\cos\alpha a\end{cases}$$

驻波

$$\text{对应的导数} \rightarrow \begin{cases} \psi'(x) = A_1 \beta e^{\beta x} & x < -a, \\ \psi'(x) = i\alpha A_0 e^{i\alpha x} - i\alpha B_0 e^{-i\alpha x} & -a < x < a \\ \psi'(x) = -\beta A_2 e^{-\beta x} & x > a \end{cases}$$

$$\begin{bmatrix} x = -a \\ x = a \end{bmatrix} \rightarrow \begin{cases} \psi'(-a) = A_1 \beta e^{-\beta a} \\ \psi'(-a) = i\alpha A_0 e^{-ia\alpha} - i\alpha B_0 e^{ia\alpha} \\ \psi'(a) = i\alpha A_0 e^{i\alpha a} - i\alpha B_0 e^{-i\alpha a} \\ \psi'(a) = -\beta A_2 e^{-\beta a} \end{cases} \rightarrow \begin{cases} A_1 \beta e^{-\beta a} = i\alpha A_0 e^{-ia\alpha} - i\alpha A_0 e^{ia\alpha} = -\alpha 2 \sin \alpha a \\ -\beta A_2 e^{-\beta a} = i\alpha A_0 e^{i\alpha a} - i\alpha A_0 e^{-i\alpha a} = -\alpha A_0 2 \sin a\alpha \end{cases}$$

$$\begin{cases} \begin{cases} A_1 e^{-\beta a} = A_0 e^{-i\alpha a} + B_0 e^{i\alpha a} = 2A_0 \cos \alpha a \\ A_2 e^{-\beta a} = A_0 e^{i\alpha a} + B_0 e^{-i\alpha a} = 2A_0 \cos \alpha a \end{cases} \\ \begin{cases} A_1 \beta e^{-\beta a} = i\alpha A_0 e^{-ia\alpha} - i\alpha A_0 e^{ia\alpha} = -\alpha 2A_0 \sin \alpha a \\ -\beta A_2 e^{-\beta a} = i\alpha A_0 e^{i\alpha a} - i\alpha A_0 e^{-i\alpha a} = -\alpha A_0 2 \sin a\alpha \end{cases} \end{cases}$$

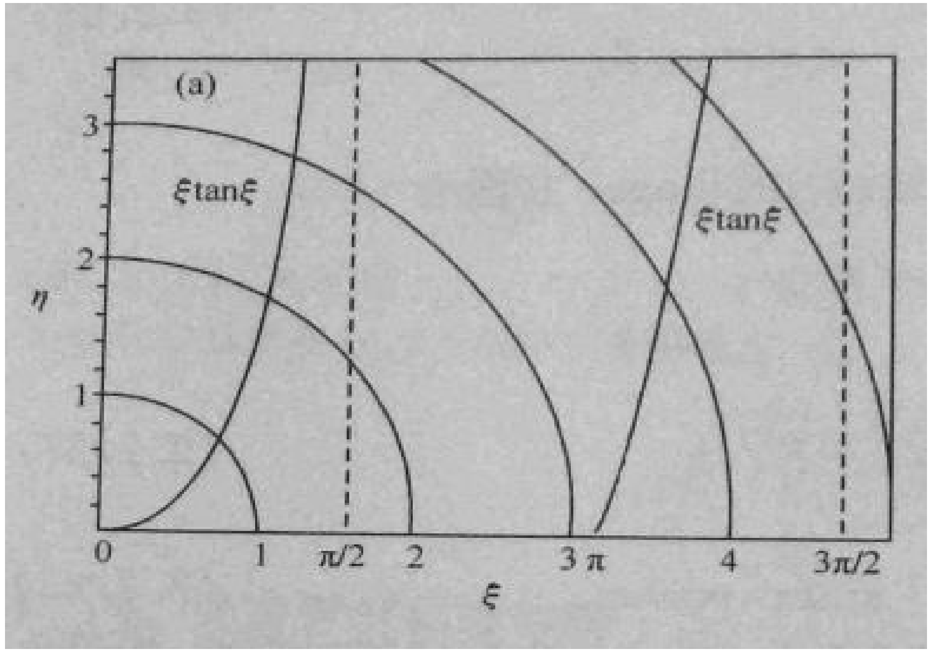
$$\rightarrow \begin{cases} \cos \alpha a = -\dfrac{\alpha \sin \alpha a}{\beta} \\ \cos \alpha a = \dfrac{\alpha \sin a\alpha}{\beta} \end{cases} \rightarrow \text{能量本质方程} \rightarrow \tan \alpha a = \pm \frac{\beta}{a}$$

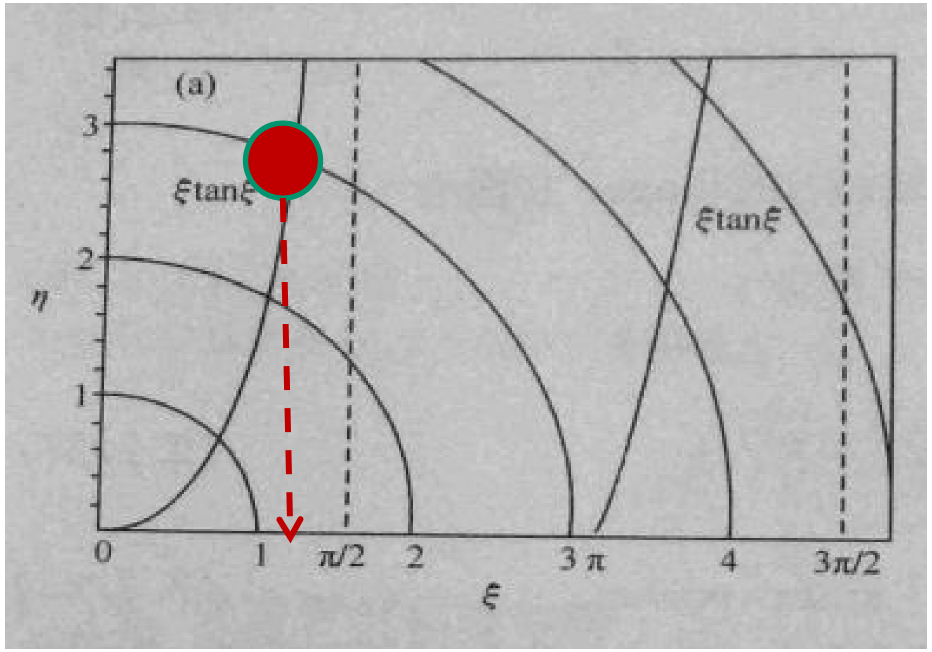
能量本质方程 $\rightarrow \tan\alpha a = \pm\dfrac{\beta}{a}$

$$\begin{cases} \alpha = \sqrt{\dfrac{2m_0}{\hbar^2}E_x} \\ \beta = \sqrt{\dfrac{2m_0}{\hbar^2}\left(U_0 - E_x\right)} \end{cases} \rightarrow \alpha^2 + \beta^2 = \frac{2m_0}{\hbar^2}U_0$$

令 $\xi = ka, \eta = \beta a \rightarrow$ 代入 $\begin{cases} \tan\alpha a = \pm\dfrac{\beta}{a} \\ \alpha^2 + \beta^2 = \dfrac{2m_0}{\hbar^2}U_0 \end{cases} \rightarrow$ 得 $\begin{cases} \eta = \xi\tan\xi \\ \xi^2 + \eta^2 = \dfrac{2m_0}{\hbar^2}U_0 a^2 \end{cases}$

$\begin{cases} \eta = \xi\tan\xi \\ \xi^2 + \eta^2 = \dfrac{2m_0}{\hbar^2}U_0 a^2 \end{cases} \rightarrow$ 作图法





假如：$R^2=\xi^2+\eta^2=\dfrac{2m_0}{\hbar^2}U_0a^2=9$

$$\rightarrow\begin{cases}\xi=1.35\\ \eta=2.75\end{cases}$$

本征能量 $\rightarrow E=\dfrac{\hbar^2}{2m_0}\left(\dfrac{1.35}{a}\right)^2$

$$\begin{cases}\beta=\dfrac{\eta}{a}\\ \alpha=\dfrac{\xi}{a}\end{cases}\Longrightarrow\begin{cases}\psi(x)=A_1e^{\beta x}\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x}\\ \psi(x)=A_2e^{-\beta x}\end{cases}\rightarrow\begin{cases}\psi(x)=-A_2e^{\frac{\eta}{a}x} & x<-a,\\ \psi(x)=A_0e^{i\frac{\xi}{a}x}+B_0e^{-i\frac{\xi}{a}x} & -a<x<a\\ \psi(x)=A_2e^{-\frac{\eta}{a}x} & x>a\end{cases}$$

$$\begin{cases}\beta=\dfrac{\eta}{a}\\[2ex] \alpha=\dfrac{\xi}{a}\end{cases}\rightarrow\begin{cases}\begin{cases}A_1e^{-\beta a}=A_0e^{-i\alpha a}+B_0e^{i\alpha a}=2A_0\cos\alpha a\\ A_2e^{-\beta a}=A_0e^{i\alpha a}+B_0e^{-i\alpha a}=2A_0\cos\alpha a\end{cases}\\ \begin{cases}A_1\beta e^{-\beta a}=i\alpha A_0e^{-ia\alpha}-i\alpha A_0e^{ia\alpha}=-\alpha 2A_0\sin\alpha a\\ -\beta A_2e^{-\beta a}=i\alpha A_0e^{i\alpha a}-i\alpha A_0e^{-i\alpha a}=-\alpha A_0 2\sin a\alpha\end{cases}\end{cases}\rightarrow\begin{cases}\begin{cases}A_1e^{-\frac{\eta}{a}a}=2A_0\cos\dfrac{\xi}{a}a=\\ A_2e^{-\frac{\eta}{a}a}=2A_0\cos\xi\end{cases}\\ \begin{cases}A_1\beta e^{-\frac{\eta}{a}a}=-\alpha 2A_0\sin\xi\\ -\beta A_2e^{-\frac{\eta}{a}a}=-\alpha A_0 2\sin\xi\end{cases}\end{cases}\rightarrow A_1=A_2=2A_0e^{-\eta}\cos\xi$$

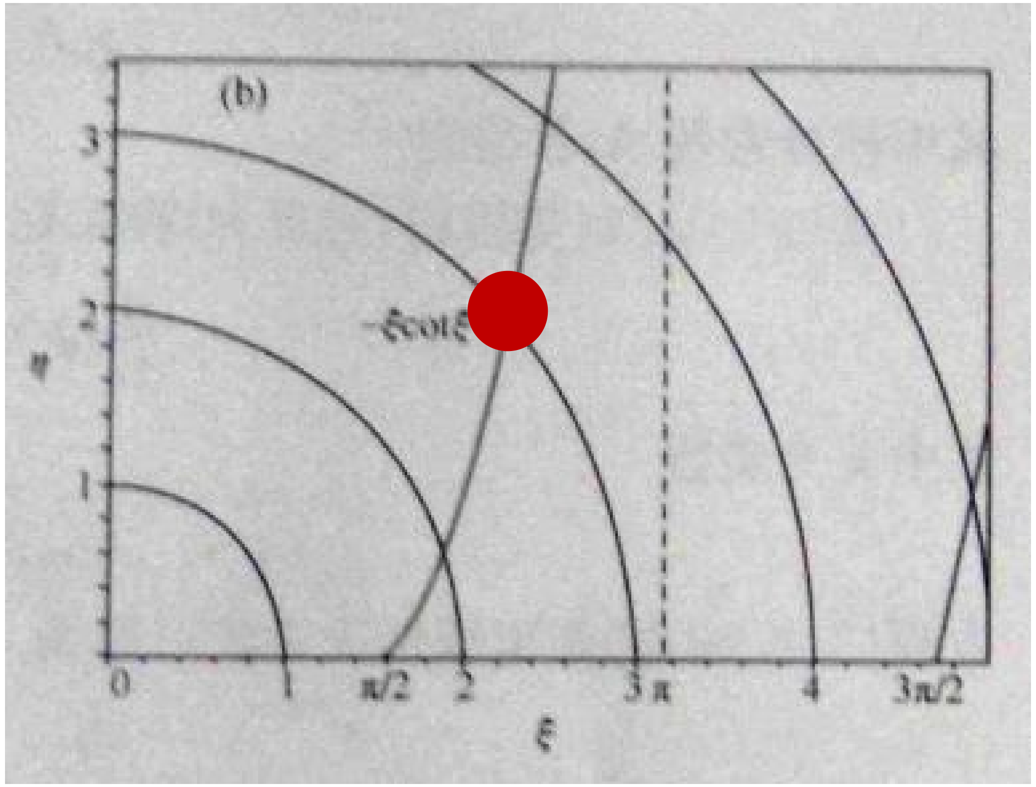
$$\text{波函数}\rightarrow\begin{cases}\psi(x)=-2A_0e^{-\eta}\cos\xi e^{\frac{\eta}{a}x} & x<-a,\\ \psi(x)=A_0e^{i\frac{\xi}{a}x}+A_0e^{-i\frac{\xi}{a}x} & -a<x<a\\ \psi(x)=2A_0e^{-\eta}\cos\xi e^{-\frac{\eta}{a}x} & x>a\end{cases}$$

如果波函数有初相位，导致

$$
\begin{cases}
\begin{cases}
A_1 e^{-\beta a} = A_0 e^{-i\alpha a} + B_0 e^{i\alpha a} = i2A_0 \sin\alpha a \\
A_2 e^{-\beta a} = A_0 e^{i\alpha a} + B_0 e^{-i\alpha a} = i2A_0 \sin\alpha a
\end{cases} \\
\begin{cases}
A_1 \beta e^{-\beta a} = i\alpha A_0 e^{-ia\alpha} - i\alpha A_0 e^{ia\alpha} = -i\alpha 2A_0 \cos\alpha a \\
-\beta A_2 e^{-\beta a} = i\alpha A_0 e^{i\alpha a} - i\alpha A_0 e^{-i\alpha a} = -i\alpha A_0 2\cos a\alpha
\end{cases}
\end{cases}
$$

$$
\rightarrow \begin{cases}
\sin\alpha a = -\dfrac{\alpha\cos\alpha a}{\beta} \\
\sin\alpha a = \dfrac{\alpha\cos a\alpha}{\beta}
\end{cases}
\rightarrow \text{能量本质方程} \rightarrow (ctg)\cot\alpha a = \pm\frac{\beta}{a}
$$

$$
\text{令}\ \xi = ka, \eta = \beta a \rightarrow \text{代入} \begin{cases}
\cot\alpha a = \pm\dfrac{\beta}{a} \\
\alpha^2 + \beta^2 = \dfrac{2m_0}{\hbar^2} U_0
\end{cases}
\rightarrow \text{得} \begin{cases}
\eta = \xi\cot\xi \\
\xi^2 + \eta^2 = \dfrac{2m_0}{\hbar^2} U_0 a^2
\end{cases}
$$



假如：$R^2=\xi^2+\eta^2=\frac{2m_0}{\hbar^2}U_0a^2=9$

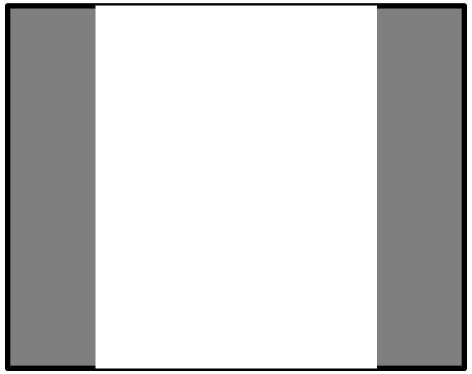
$$\rightarrow\begin{cases}\xi=2.35\\ \eta=1.90\end{cases}$$

本征能量 $\rightarrow E=\frac{\hbar^2}{2m_0}\left(\frac{2.35}{a}\right)^2$

$$\begin{cases}\eta=\xi\cot\xi\\ \xi^2+\eta^2=\frac{2m_0}{\hbar^2}U_0a^2\end{cases}$$

波函数 $\rightarrow\begin{cases}\psi(x)=-2A_0e^{-\eta}\sin\xi e^{\frac{\eta}{a}x} & x<-a,\\ \psi(x)=A_0e^{i\frac{\xi}{a}x}-A_0e^{-i\frac{\xi}{a}x} & -a<x<a\\ \psi(x)=2A_0e^{-\eta}\sin\xi e^{-\frac{\eta}{a}x} & x>a\end{cases}$

3.一维有限深方势阱（二）



$$\left(-\frac{\hbar^2 d^2}{2mdx^2}+U_x\right)\psi(x)=E_x\psi(x)$$

$$\begin{cases}\psi(x)=A_1e^{\beta x} & x<-a,\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x} & -a<x<a\\ \psi(x)=A_2e^{-\beta x} & x>a\end{cases}\to\begin{cases}a=\sqrt{\dfrac{2m_0}{\hbar^2}E_x}\\ \beta=\sqrt{\dfrac{2m_0}{\hbar^2}\left(U_0-E_x\right)}\end{cases}$$

$$\begin{cases}\psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x}\\ \psi'(x)=i\alpha A_0e^{i\alpha x}-i\alpha B_0e^{-i\alpha x}\end{cases}\quad\begin{bmatrix}x=-a\\ x=a\end{bmatrix}\to\begin{cases}\begin{cases}\psi(-a)=A_0e^{-i\alpha a}+B_0e^{i\alpha a}\\ \psi'(-a)=i\alpha A_0e^{-i\alpha a}-i\alpha B_0e^{i\alpha a}\end{cases}\\ \begin{cases}\psi(a)=A_0e^{i\alpha a}+B_0e^{-i\alpha a}\\ \psi'(a)=i\alpha A_0e^{i\alpha a}-i\alpha B_0e^{-i\alpha a}\end{cases}\end{cases}$$

矩阵 $\to\begin{bmatrix}\psi(-a)\\ \psi'(-a)\end{bmatrix}=\begin{bmatrix}e^{-i\alpha a} & e^{i\alpha a}\\ i\alpha e^{-i\alpha a} & -i\alpha e^{i\alpha a}\end{bmatrix}\begin{bmatrix}A_0\\ B_0\end{bmatrix}$

$$\begin{cases}A_0=\dfrac{i\alpha\psi(a)+\psi'(a)}{2i\alpha}e^{-i\alpha a}\\ B_0=\dfrac{i\alpha\psi(a)-\psi'(a)}{2i\alpha}e^{i\alpha a}\end{cases}\to\begin{bmatrix}A_0\\ B_0\end{bmatrix}=\frac{1}{2i\alpha}\begin{bmatrix}i\alpha e^{-i\alpha a} & e^{-i\alpha a}\\ i\alpha e^{i\alpha a} & -e^{i\alpha a}\end{bmatrix}\begin{bmatrix}\psi(a)\\ \psi'(a)\end{bmatrix}$$

$$\begin{bmatrix}\psi(-a)\\ \psi'(-a)\end{bmatrix}=\begin{bmatrix}e^{-i\alpha a} & e^{i\alpha a}\\ i\alpha e^{-i\alpha a} & -i\alpha e^{i\alpha a}\end{bmatrix}\begin{bmatrix}A_0\\ B_0\end{bmatrix}\qquad \begin{bmatrix}A_0\\ B_0\end{bmatrix}=\frac{1}{2i\alpha}\begin{bmatrix}i\alpha e^{-i\alpha a} & e^{-i\alpha a}\\ i\alpha e^{i\alpha a} & -e^{i\alpha a}\end{bmatrix}\begin{bmatrix}\psi(a)\\ \psi'(a)\end{bmatrix}$$

$$\to\begin{bmatrix}\psi(-a)\\ \psi'(-a)\end{bmatrix}=\frac{1}{2i\alpha}\begin{bmatrix}e^{-i\alpha a} & e^{i\alpha a}\\ i\alpha e^{-i\alpha a} & -i\alpha e^{i\alpha a}\end{bmatrix}\begin{bmatrix}i\alpha e^{-i\alpha a} & e^{-i\alpha a}\\ i\alpha e^{i\alpha a} & -e^{i\alpha a}\end{bmatrix}\begin{bmatrix}\psi(a)\\ \psi'(a)\end{bmatrix}$$

展开 $\to\begin{bmatrix}\psi(-a)\\ \psi'(-a)\end{bmatrix}=\frac{1}{2i\alpha}\begin{bmatrix}\psi(a)\\ \psi'(a)\end{bmatrix}\begin{bmatrix}i\alpha e^{-2i\alpha a}+i\alpha e^{2i\alpha a} & e^{-2i\alpha a}-e^{2i\alpha a}\\ -\alpha^2 e^{-2i\alpha a}+\alpha^2 e^{2i\alpha a} & i\alpha e^{-2i\alpha a}+i\alpha e^{2i\alpha a}\end{bmatrix}\begin{bmatrix}\psi(a)\\ \psi'(a)\end{bmatrix}$

化简 $\to\begin{bmatrix}\psi(-a)\\ \psi'(-a)\end{bmatrix}=\frac{1}{\alpha}\begin{bmatrix}\cos 2\alpha a & -\frac{1}{a}\sin 2\alpha a\\ \alpha\sin 2\alpha a & \cos 2\alpha a\end{bmatrix}\begin{bmatrix}\psi(a)\\ \psi'(a)\end{bmatrix}$

$$\begin{cases}\psi(x)=A_1e^{\beta x} & x<-a,\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x} & -a<x<a\\ \psi(x)=A_2e^{-\beta x} & x>a\end{cases}\quad\to\quad\begin{cases}\begin{cases}\psi(-a)=A_1e^{-a\beta}\\ \psi'(-a)=A_1\beta e^{a\beta}\end{cases}\\ \begin{cases}\psi(a)=A_2e^{-\beta a}\\ \psi'(a)=-\beta A_2e^{-\beta a}\end{cases}\end{cases}$$

$$\rightarrow \begin{cases} \begin{cases} \psi(-a) = A_1 e^{-a\beta} \\ \psi'(-a) = A_1 \beta e^{-a\beta} \end{cases} \\ \begin{cases} \psi(a) = A_2 e^{-\beta a} \\ \psi'(a) = -\beta A_2 e^{-\beta a} \end{cases} \end{cases} \qquad \begin{bmatrix} x = -a \\ x = a \end{bmatrix} \rightarrow \begin{cases} \begin{bmatrix} \psi(-a) \\ \psi'(-a) \end{bmatrix} = A_1 e^{-a\beta} \begin{bmatrix} 1 \\ \beta \end{bmatrix} \\ \begin{bmatrix} \psi(a) \\ \psi'(a) \end{bmatrix} = A_2 e^{-\beta a} \begin{bmatrix} 1 \\ -\beta \end{bmatrix} \end{cases}$$

$$\begin{bmatrix} \psi(-a) \\ \psi'(-a) \end{bmatrix} = \frac{1}{\alpha} \begin{bmatrix} \cos 2\alpha a & -\frac{1}{a}\sin 2\alpha a \\ \alpha \sin 2\alpha a & \cos 2\alpha a \end{bmatrix} \begin{bmatrix} \psi(a) \\ \psi'(a) \end{bmatrix} \rightarrow A_1 e^{-a\beta} \begin{bmatrix} 1 \\ \beta \end{bmatrix} = \frac{A_2 e^{-a\beta}}{\alpha} \begin{bmatrix} \cos 2\alpha a & -\frac{1}{a}\sin 2\alpha a \\ \alpha \sin 2\alpha a & \cos 2\alpha a \end{bmatrix} \begin{bmatrix} 1 \\ -\beta \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} -\beta & 1 \end{bmatrix} \begin{bmatrix} 1 \\ \beta \end{bmatrix} = \frac{1}{\alpha} \begin{bmatrix} -\beta & 1 \end{bmatrix} \begin{bmatrix} \cos 2\alpha a & -\frac{1}{a}\sin 2\alpha a \\ \alpha \sin 2\alpha a & \cos 2\alpha a \end{bmatrix} \begin{bmatrix} 1 \\ -\beta \end{bmatrix} \rightarrow \frac{1}{\alpha} \begin{bmatrix} -\beta & 1 \end{bmatrix} \begin{bmatrix} \cos 2\alpha a & -\frac{1}{a}\sin 2\alpha a \\ \alpha \sin 2\alpha a & \cos 2\alpha a \end{bmatrix} \begin{bmatrix} 1 \\ -\beta \end{bmatrix} = 0$$

$$\rightarrow -\beta \cos 2\alpha a + \alpha \sin 2\alpha a - \frac{\beta^2}{\alpha} \sin 2\alpha a - \beta \cos 2\alpha a = 0$$

$$\rightarrow \tan 2\alpha a = \frac{2\alpha\beta}{\alpha^2 - \beta^2} \qquad \rightarrow \frac{2\tan \alpha a}{1 - \tan^2 \alpha\alpha} = \frac{2\alpha\beta}{\alpha^2 - \beta^2}$$

$$\rightarrow 2\alpha\beta - 2\alpha\beta \tan^2 \alpha\alpha = 2\alpha^2 \tan \alpha a - 2\beta^2 \tan \alpha a$$

$$\rightarrow 2\alpha\beta - 2\alpha\beta\tan^2\alpha a = 2\alpha^2\tan\alpha a - 2\beta^2\tan\alpha a$$

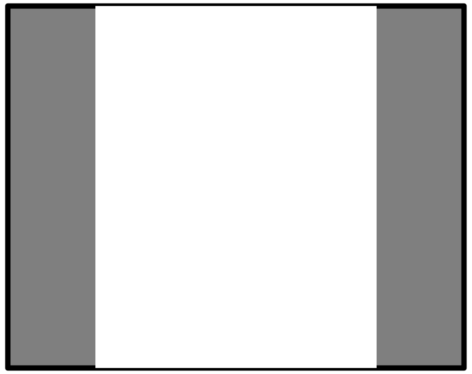
$$\rightarrow \alpha\beta\tan^2\alpha a + \alpha^2\tan\alpha a - \beta^2\tan\alpha a - \alpha\beta = 0$$

$$\tan\alpha a = \frac{-\left(\alpha^2-\beta^2\right) \pm \sqrt{\left(\alpha^2-\beta^2\right)^2 + 4\alpha^2\beta^2}}{2\alpha\beta} = \frac{\beta}{a}$$

$$\begin{cases} a = \sqrt{\dfrac{2m_0}{\hbar^2}E_x} \\ \beta = \sqrt{\dfrac{2m_0}{\hbar^2}\left(U_0 - E_x\right)} \end{cases}$$

$$令\xi = ka, \eta = \beta a \rightarrow 代入 \begin{cases} \cot\alpha a = \pm\dfrac{\beta}{a} \\ \alpha^2 + \beta^2 = \dfrac{2m_0}{\hbar^2}U_0 \end{cases} \rightarrow 得 \begin{cases} \eta = \xi\cot\xi \\ \xi^2 + \eta^2 = \dfrac{2m_0}{\hbar^2}U_0 a^2 \end{cases}$$

$$波函数 \rightarrow \begin{cases} \psi(x) = -2A_0 e^{-\eta}\sin\xi e^{\frac{\eta}{a}x} & x < -a, \\ \psi(x) = A_0 e^{i\frac{\xi}{a}x} - A_0 e^{-i\frac{\xi}{a}x} & -a < x < a \\ \psi(x) = 2A_0 e^{-\eta}\sin\xi e^{-\frac{\eta}{a}x} & x > a \end{cases}$$

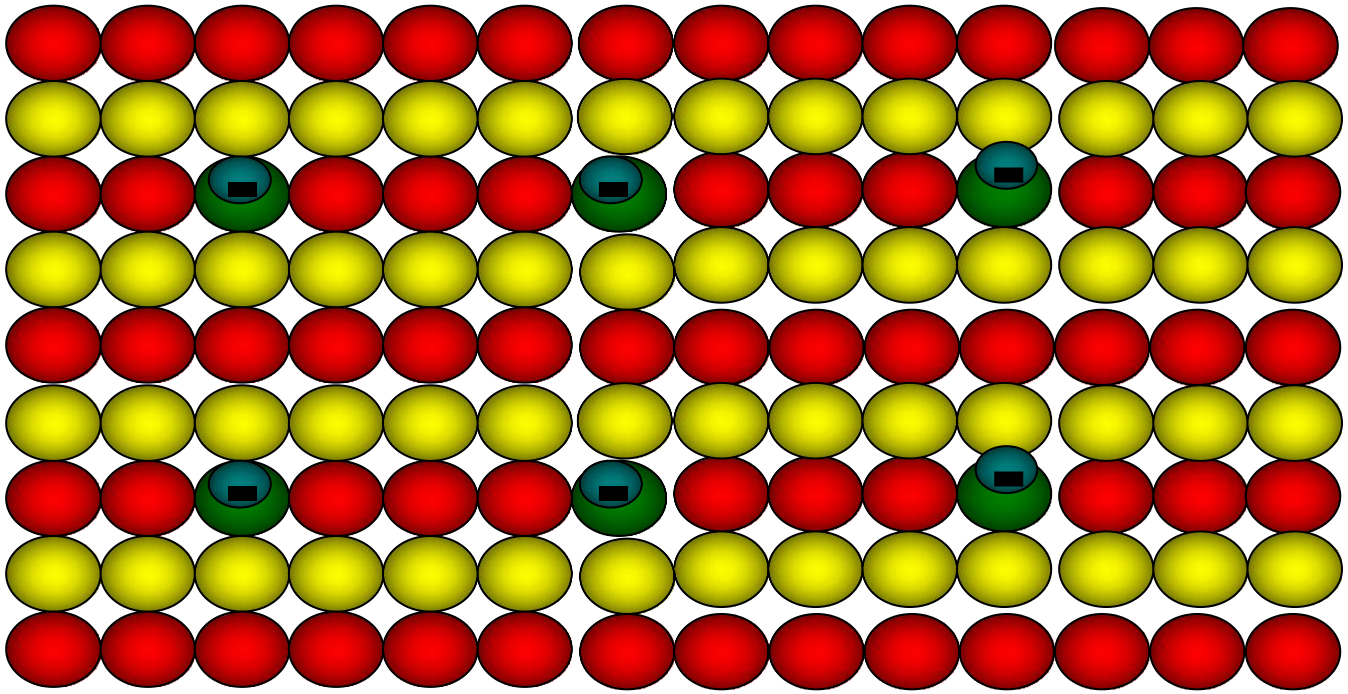


$$解集 \rightarrow \begin{cases} f\left(E\right) = \tan \alpha a = \tan \sqrt{\dfrac{2m_0}{\hbar^2} E_x} \alpha \\ f\left(E\right) = \dfrac{\sqrt{\left(U_0 - E_x\right)}}{\sqrt{E_x}} \end{cases}$$

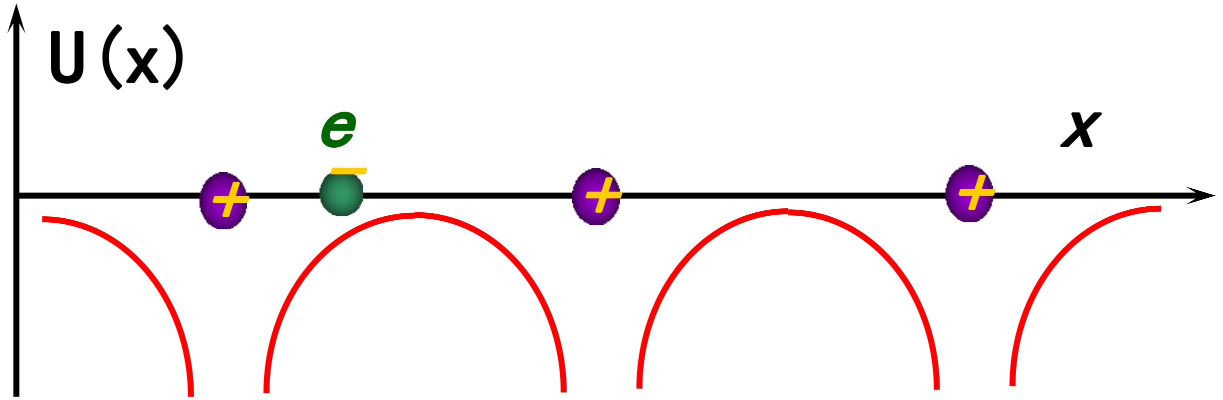
$$得本质波函数 \rightarrow \begin{cases} \psi(x) = A_1 e^{\beta x} & x < -a, \\ \psi(x) = A_0 e^{i\alpha x} + B_0 e^{-i\alpha x} & -a < x < a \\ \psi(x) = A_2 e^{-\beta x} & x > a \end{cases}$$

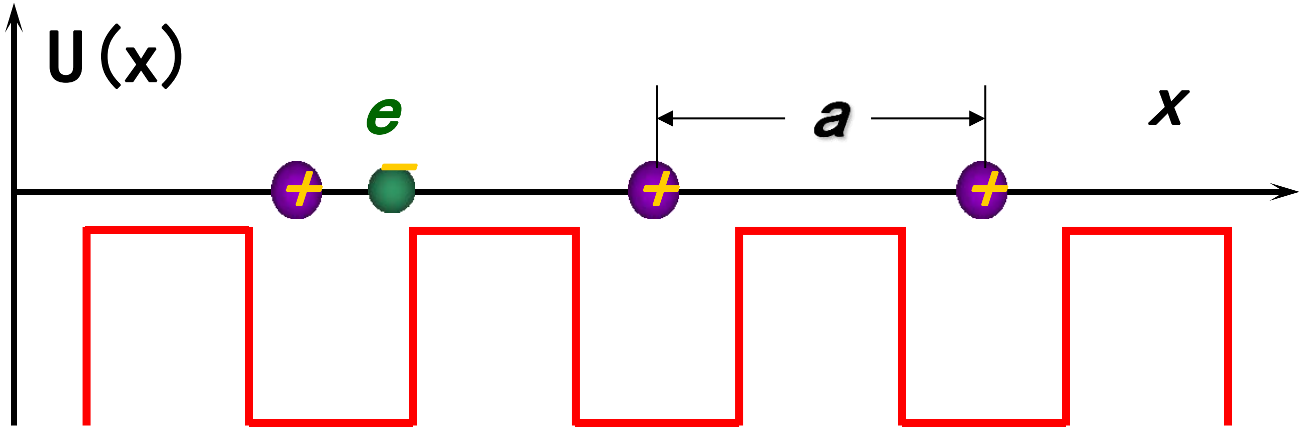
$$归一化条件 \rightarrow \begin{cases} \psi(x) = A_1 e^{\beta x} & x < -a, \\ \psi(x) = A_0 e^{i\alpha x} + B_0 e^{-i\alpha x} & -a < x < a \\ \psi(x) = A_2 e^{-\beta x} & x > a \end{cases}$$

4. 半导体的能带理论



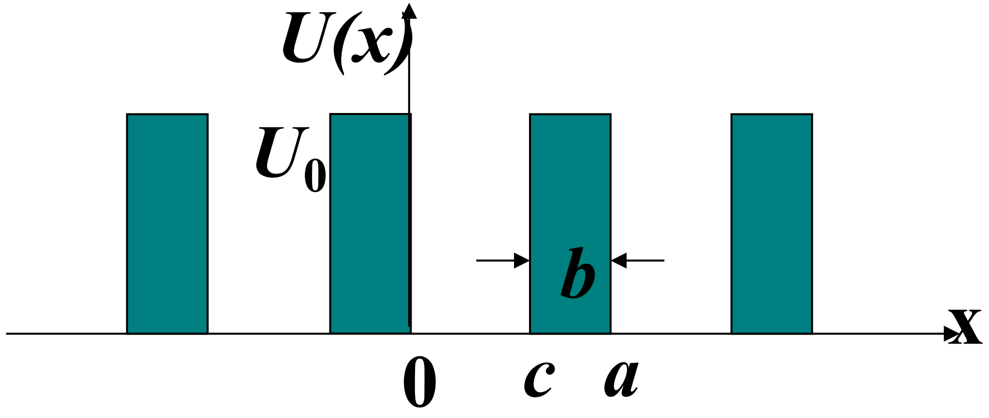
● 简单物理模型





粒子处在一维周期性方势阱中的运动

$$U(x)=\begin{cases}0 & (0<x<c)\\ U_0 & (c\le x\le a)\end{cases}\qquad a=b+c$$



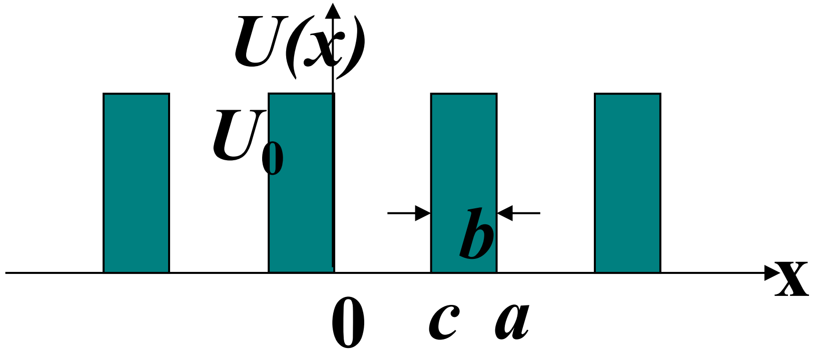
$$\rightarrow U\left(x\right)=U\left(x+a\right)$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right)\Phi(x)=E\Phi(x)\qquad U\left(x\right)=U\left(x+a\right)\rightarrow\Phi(x)=e^{ikx}u\left(x\right)$$

$$U\left(x\right)=0\quad(0<c)\rightarrow\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\Phi\left(x\right)=E\Phi\left(x\right)$$

$$\Phi\left(x\right)=e^{ikx}u\left(x\right)\text{代入}\rightarrow\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\Phi\left(x\right)=E\Phi\left(x\right)\text{得}\rightarrow\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\left(\alpha^2-k^2\right)u\left(x\right)=0$$

$$\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\left(\alpha^2-k^2\right)u(x)=0$$



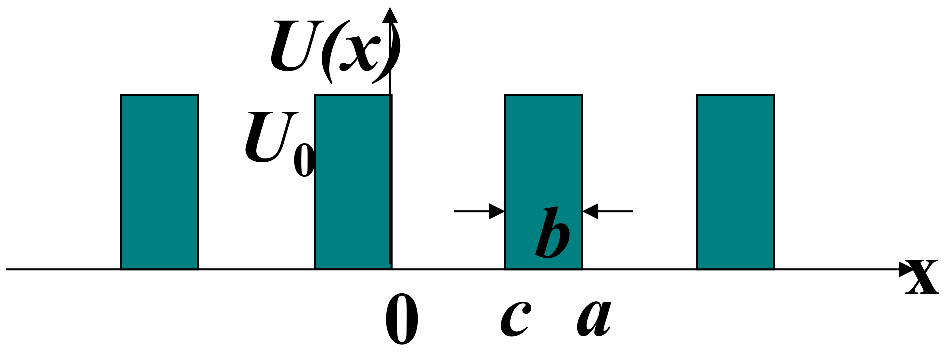
令$\alpha^2=\frac{2mE}{\hbar^2}$得解$\rightarrow u(x)=A_0e^{i(\alpha-k)x}+B_0e^{-i(\alpha+k)x}$

$$U(x)=U_0\quad(c\le x\le a)\rightarrow\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right)\Phi(x)=E\Phi(x)$$

试探解$\Phi_1(x)=e^{ikx}u(x)$代入上式得$\rightarrow\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-\left(\beta^2+k^2\right)u(x)=0$

$\beta^2=\frac{2m}{\hbar^2}(U_0-E)\rightarrow$代入上式得$\rightarrow u(x)=C_0e^{(\beta-ik)x}+D_0e^{-(\beta+ik)x}$

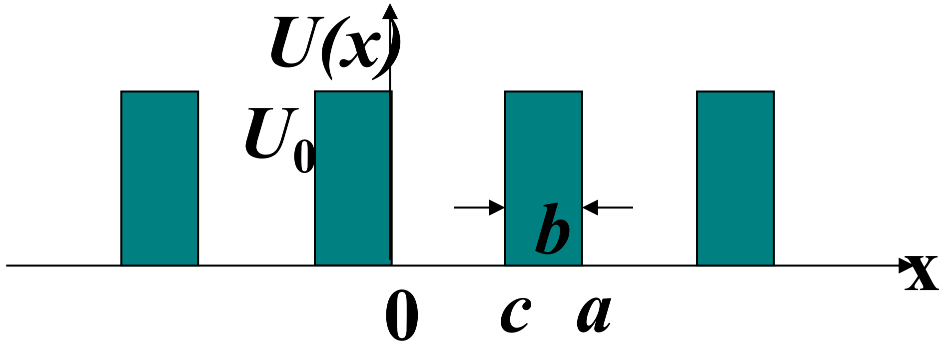
$$\begin{cases} u(x) = A_0 e^{i(\alpha-k)x} + B_0 e^{-i(\alpha+k)x} & U=0 \\ u(x) = C_0 e^{(\beta-ik)x} + D_0 e^{-(\beta+ik)x} & U=U_0 \end{cases}$$



$$\text{周期性} \rightarrow \begin{cases} u(x+na) = A_n e^{i(\alpha-k)(x+na)} + B_n e^{-i(\alpha+k)(x+na)} \\ u(x+na) = C_n e^{(\beta-ik)(x+na)} + D_n e^{-(\beta+ik)(x+na)} \end{cases}$$

$$\rightarrow \begin{cases} A_n = A_0 e^{-i(\alpha-k)(na)} \\ B_n = B_0 e^{i(\alpha+k)(na)} \\ C_n = C_0 e^{-(\beta-ik)(na)} \\ D_n = D_0 e^{(\beta+ik)(na)} \end{cases}$$

$$x=0\rightarrow\begin{cases}u(x)=A_0e^{i(\alpha-k)x}+B_0e^{i(\alpha+k)x}\\ u(x)=C_0e^{(\beta-ik)x}+D_0e^{-(\beta+ik)x}\end{cases}$$



连续条件（含导数连续条件）$\rightarrow\begin{cases}A_0+B_0=C_0+D_0\\ i(\alpha-k)A_0-i(\alpha+k)B_0=(\beta-ik)C_0-(\beta+ik)D_0\end{cases}$

$$x=c\rightarrow\begin{cases}A_0e^{i(\alpha-k)c}+B_0e^{-i(\alpha+k)c}=C_1e^{(\alpha-ik)c}+D_1e^{-(\alpha+ik)c}=C_0e^{(\alpha-ik)c}+D_0e^{-(\alpha+ik)c}\\ i(\alpha-k)A_0e^{i(\alpha-k)c}-i(\alpha+k)B_0e^{-i(\alpha+k)c}=(\beta-ik)C_0e^{-(\beta-ik)c}-(\beta+ik)D_0e^{(\beta+ik)c}\end{cases}$$

$$\rightarrow\begin{cases}A_0+B_0-C_0-D_0=0\\ i(\alpha-k)A_0-i(\alpha+k)B_0-(\beta-ik)C_0+(\alpha+ik)D_0=0\\ A_0e^{i(\alpha-k)c}+B_0e^{-i(\alpha+k)c}-C_0e^{-(\beta-ik)b}-D_0e^{(\beta+ik)b}=0\\ i(\alpha-k)A_0e^{i(\alpha\text{-}k)c}-i(\alpha+k)B_0e^{-i(\alpha+k)c}\\ -(\beta-ik)C_0e^{-(\beta-ik)b}+(\beta+ik)D_0e^{(\beta+ik)b}=0\end{cases}$$

系数有解的前提: $\begin{vmatrix}1 & 1 & -1 & -1\\ i(\alpha-k) & -i(\alpha+k) & -(\beta-ik) & (\alpha+ik)\\ e^{i(\alpha-k)c} & -e^{-i(\alpha+k)c} & -e^{i(\alpha+k)b} & -e^{-i(\alpha-k)b}\\ i(\alpha-k)e^{i(\alpha-k)c} & -(\alpha+k)e^{-i(\alpha+k)c} & -(\beta-ik)e^{-(\beta-ik)b} & (\beta+ik)e^{(\beta+ik)b}\end{vmatrix}=0$

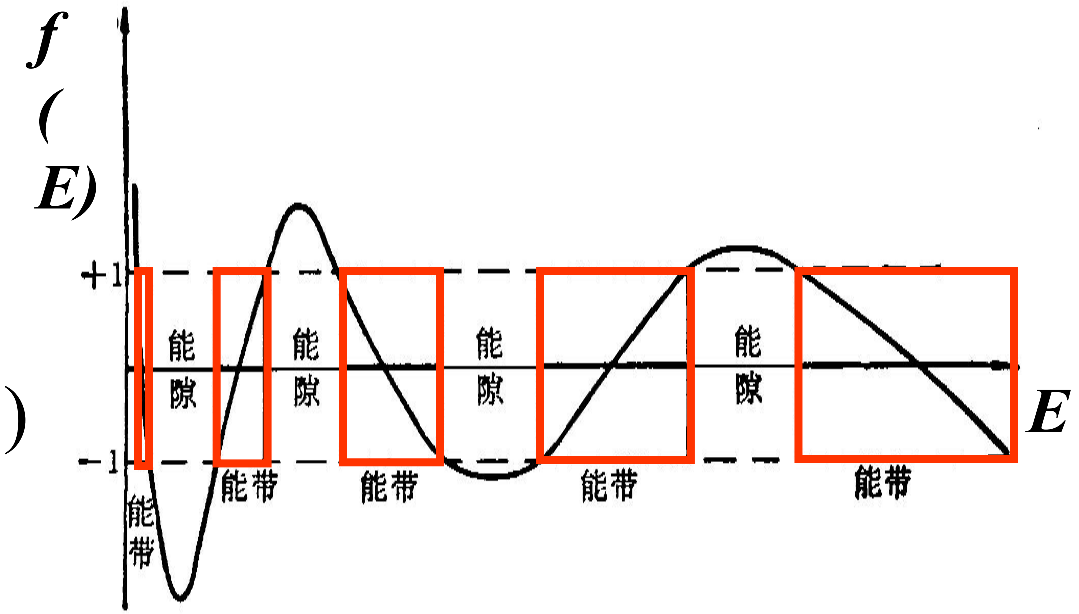
$$\rightarrow\frac{\beta^2-\alpha^2}{2\alpha\beta}\sinh\beta b\sin\alpha c+\cosh\beta b\cos ac=\cos(ka)$$

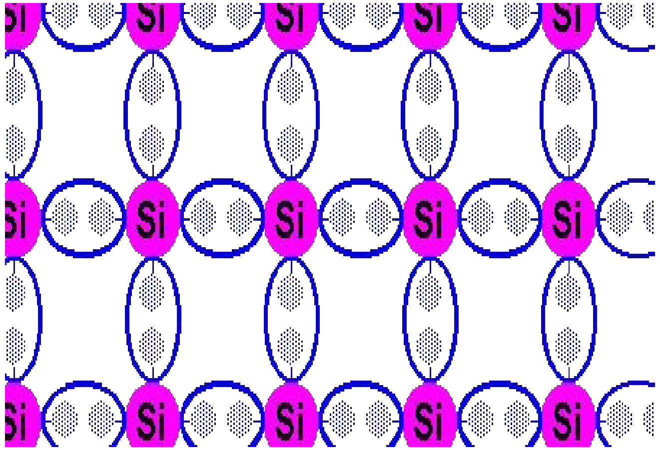
$U_0\rightarrow\infty, b\rightarrow 0$进行简化后得 $\rightarrow\left(\frac{maU_0b}{\hbar^2}\right)\frac{\sin(\beta a)}{\beta a}+\cos(\beta a)=\cos(ka)$

$$\left(\frac{maU_0b}{\hbar^2}\right)\frac{\sin(\beta a)}{\beta a}+\cos(\beta a)=\cos(ka)$$

$$\begin{cases}\alpha^2=\dfrac{2mE}{h^2}\\[2ex] \beta^2=\dfrac{2m}{h^2}(U_0-E)\end{cases}$$

$$\rightarrow\begin{cases}f(E)=\left(\dfrac{maU_0b}{\hbar^2}\right)\dfrac{\sin(\beta a)}{\beta a}+\cos(\beta a)\\[2ex] f(E)=\cos(ka)\end{cases}$$

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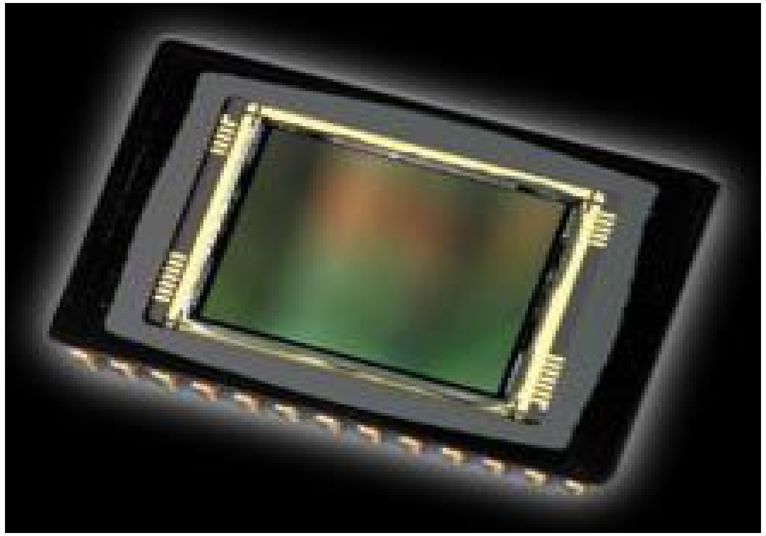
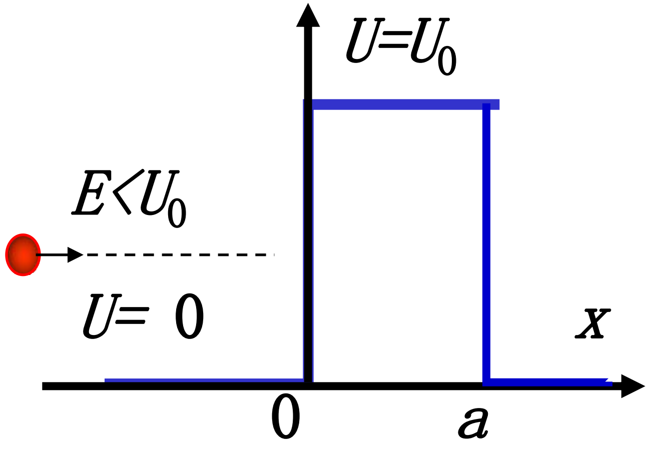


5. 隧道效应（势垒贯穿）

（1）自由粒子处遇到的势是有限高和有限宽的势垒：



$$U(x)=\begin{cases}U_0, & 0<x<a\\ 0, & x<0,x>a\end{cases}$$

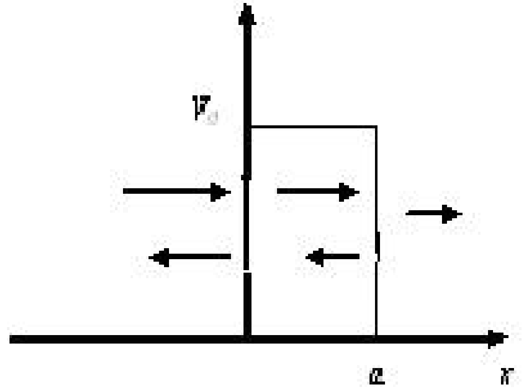
解：

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+U(x)\psi(x)=E\psi(x)\qquad \begin{cases}\psi_1''+k^2\psi_1=0 & x<0 & I\ 区\\ \psi_2''+k'^2\psi_2=0 & 0<x<a & II\ 区\\ \psi_3''+k^2\psi_3=0 & x>a & III\ 区\end{cases}$$

$$\begin{cases}k=\sqrt{\dfrac{2mE}{\hbar^2}}\\ k'=\sqrt{\dfrac{2m(E-U_0)}{\hbar^2}}\end{cases}\rightarrow\begin{cases}\psi_1(x)=Ae^{+ikx}+Be^{-ikx}\\ \psi_2(x)=De^{-ik'x}+Fe^{+ik'x} & 0\le x\le a\\ \psi_3(x)=Ce^{+ikx}\end{cases}$$

（2）确定系数

利用波函数及微商连续条件



$$\rightarrow\begin{cases}\psi_1(x)=Ae^{+ikx}+Be^{-ikx}\\ \psi_2(x)=De^{-k'x}+Fe^{+k'x} \quad 0\le x\le a\end{cases}\rightarrow\begin{cases}\psi_1(0)=Ae^{+ik0}+Be^{-ik0}\\ \psi_2(0)=De^{-ik'0}+Fe^{+ik'0} \quad 0\le x\le a\end{cases}$$

$$\begin{cases}\psi_1(0)=\psi_2(0)\\ \left(\dfrac{d\psi_1}{dx}\right)_{x=0}=\left(\dfrac{d\psi_2}{dx}\right)_{x=0}\end{cases}\rightarrow\begin{cases}Ae^{+ik0}+Be^{-ik0}=De^{-k'0}+Fe^{+k'0}\\ kA-kB=k'D-k'F\end{cases}$$

$$\rightarrow\begin{cases}\psi_2(x)=De^{-ik'x}+Fe^{+ik'x} \quad 0\le x\le a\\ \psi_3(x)=Ce^{+ikx}\end{cases}\quad\begin{cases}(\psi_2)_{x=a}=(\psi_3)_{x=a}\\ \left(\dfrac{d\psi_2}{dx}\right)_{x=a}=\left(\dfrac{d\psi_3}{dx}\right)_{x=a}\end{cases}\rightarrow\begin{cases}De^{ik'a}+Fe^{-ik'a}=Ce^{ika}\\ k'De^{ik'a}-k'Fe^{-ik'a}=kCe^{ika}\end{cases}$$

$$\begin{cases} A+B=D+F \\ kA-kB=k'D-k'F \\ De^{ik'a}+Fe^{-ik'a}=Ce^{ika} \\ k'De^{ik'a}-k'Fe^{-ik'a}=kCe^{ika} \end{cases}$$

$$\rightarrow \begin{cases} C=\dfrac{4kk'e^{-ika}}{(k+k')^2e^{-ik'a}-(k-k')^2e^{ik'a}}A \\ B=\dfrac{2i(k^2+k'^2)\sin ak'}{(k-k')^2e^{ik'a}-(k+k')^2e^{-ik'a}}A \end{cases}$$

（3）几率流密度矢量和粒子数守恒定律：

$$\rho_{几率密度}(r,t)=\psi^*(r,t)\psi(r,t)$$

$$\to\frac{\partial\rho(r,t)}{\partial t}=\psi^*(r,t)\frac{\partial\psi(r,t)}{\partial t}+\frac{\partial\psi^*(r,t)}{\partial t}\psi(r,t)$$

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)\right)\psi(x,t)\to\to\begin{cases}\dfrac{\partial\psi(r,t)}{\partial t}=\dfrac{i\hbar}{2m}\nabla^2\psi+\dfrac{1}{i\hbar}U(r)\psi\\[2ex]\dfrac{\partial\psi^*(r,t)}{\partial t}=-\dfrac{i\hbar}{2m}\nabla^2\psi^*-\dfrac{1}{i\hbar}U(r)\psi^*\end{cases}$$

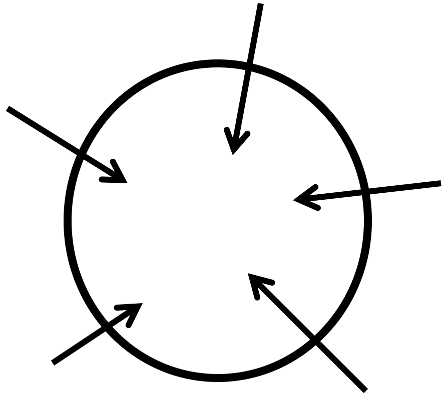
$$\to\frac{\partial\rho(r,t)}{\partial t}=\psi^*\left(\frac{i\hbar}{2m}\nabla^2\psi+\frac{1}{i\hbar}U(r)\psi\right)+\left(-\frac{i\hbar}{2m}\nabla^2\psi^*-\frac{1}{i\hbar}U(r)\psi^*\right)\psi$$

$$\to\frac{\partial\rho(r,t)}{\partial t}=\frac{i\hbar}{2m}\left(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*\right)$$

$$\rightarrow\frac{\partial\rho(r,t)}{\partial t}=\frac{i\hbar}{2m}\left(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*\right)$$

$$\nabla\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)=\left(\nabla\psi^*\nabla\psi+\psi^*\nabla^2\psi-\nabla\psi\nabla\psi^*-\nabla\psi\nabla^2\psi^*\right)=\left(\psi^*\nabla^2\psi-\nabla\psi\nabla^2\psi^*\right)$$

$$\rightarrow\frac{\partial\rho(r,t)}{\partial t}=\frac{i\hbar}{2m}\vec{\nabla}\bullet\left(\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*\right)$$



$$令J=\frac{i\hbar}{2m}\left(\psi\nabla\psi^*-\psi^*\nabla\psi\right)\rightarrow\frac{\partial\rho(r,t)}{\partial t}+\vec{\nabla}\bullet\vec{J}=0$$

$$\int_V\frac{\partial\rho(r,t)}{\partial t}dV=\frac{d}{dt}\int_V\rho(r,t)\,dV=-\int_V\left(\vec{\nabla}\bullet\vec{J}\right)dV=-\oint\vec{J}\bullet d\vec{S}\,(高斯定律)$$

$\vec{J}$显然就是单位时间单位面积流过的粒子数

$$\rho_{\text{质量密度}}\left(r,t\right)=m\psi^{*}\left(r,t\right)\psi\left(r,t\right)$$

$$J_{\text{质量流密度}}=m\frac{i\hbar}{2m}\left(\psi\nabla\psi^{*}-\psi^{*}\nabla\psi\right)=\frac{i\hbar}{2}\left(\psi\nabla\psi^{*}-\psi^{*}\nabla\psi\right)$$

$$\frac{\partial\rho_{\text{质量密度}}\left(r,t\right)}{\partial t}+\vec{\nabla}\bullet\vec{J}_{\text{质量流密度}}=0$$

$$\rightarrow\frac{d}{dt}\int_{V}\rho_{\text{质量密度}}\left(r,t\right)dV=-\oint\vec{J}_{m}\bullet d\vec{S}\rightarrow\text{质量守恒定律}$$

$$\rightarrow\frac{d}{dt}\int_{V}\rho_{\text{电荷密度}}\left(r,t\right)dV=-\oint\vec{J}_{q}\bullet d\vec{S}\rightarrow\text{电荷守恒定律}$$

$$\psi(x)=Ae^{+ikx}\rightarrow J=\frac{i\hbar}{2m}\left(\psi\nabla\psi^{*}-\psi^{*}\nabla\psi\right)\rightarrow J=\frac{i\hbar}{2m}[Ae^{ikx}\frac{d}{dx}A^{*}e^{-ikx}-A^{*}e^{-ikx}\frac{d}{dx}Ae^{ikx}=\frac{k\hbar}{m}|A|^{2}$$

$$\begin{cases}\psi_1(x)=Ae^{+ikx}+Be^{-ikx}\\ \psi_3(x)=Ce^{+ikx}\end{cases}\rightarrow\begin{cases}J_{\text{入射波几率流密度}}=\dfrac{k\hbar}{m}|A|^{2}\\ J_{\text{反射波几率流密度}}=\dfrac{k\hbar}{m}|B|^{2}\\ J_{\text{透射波几率流密度}}=\dfrac{k\hbar}{m}|C|^{2}\end{cases}$$

$$\rightarrow\begin{cases}C=\dfrac{4kk'e^{-ika}}{(k+k')^{2}e^{-ik'a}-(k-k')^{2}e^{ik'a}}A\\ B=\dfrac{2i(k^{2}+k'^{2})\sin ak'}{(k-k')^{2}e^{ik'a}-(k+k')^{2}e^{-ik'a}}A\end{cases}\quad\begin{cases}T_{\text{投射系数}}=\dfrac{J_{\text{透射}}}{J_{\text{入射}}}=\dfrac{|C|^{2}}{|A|^{2}}=\dfrac{4k^{2}k'^{2}}{(k^{2}-k'^{2})^{2}\sin^{2}k'a+4k^{2}k'^{2}}\\ R_{\text{反射系数}}=\dfrac{J_{\text{反射}}}{J_{\text{入射}}}=\dfrac{|B|^{2}}{|A|^{2}}=\dfrac{(k^{2}-k'^{2})^{2}\sin^{2}k'a}{(k^{2}-k'^{2})^{2}\sin^{2}k'a+4k^{2}k'^{2}}\end{cases}$$

透射系数

$$T_{透射系数}=\frac{J_{透射}}{J_{入射}}=\frac{|C|^2}{|A|^2}=\frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2 k'a+4k^2k'^2}$$

$$\text{如果}E<<U\text{和}a\text{不太小},\rightarrow shk'a=\frac{e^{k'a}-e^{-k'a}}{2}\approx\frac{e^{k'a}}{2}$$

$$T_{透射系数}=\frac{4k^2k'^2}{(k^2+k'^2)^2sh^2k'a+4k^2k'^2}\approx\frac{4k^2k'^2}{\frac{1}{4}(k^2+k'^2)^2e^{2k'a}+4k^2k'^2}$$

$$k'=\sqrt{\frac{2m(E-U_0)}{\hbar^2}}\rightarrow k'a\text{足够大}$$

$$\rightarrow T_{透射系数}=\frac{1}{\frac{1}{16}\left(\frac{k}{k'}+\frac{k'}{k}\right)^2e^{2k'a}+1}\approx\frac{16k^2k'^2}{\left(k^2+k'^2\right)^2}e^{-2ka}=T_0e^{-\frac{2a}{\hbar}\sqrt{2m(U-E)}}$$

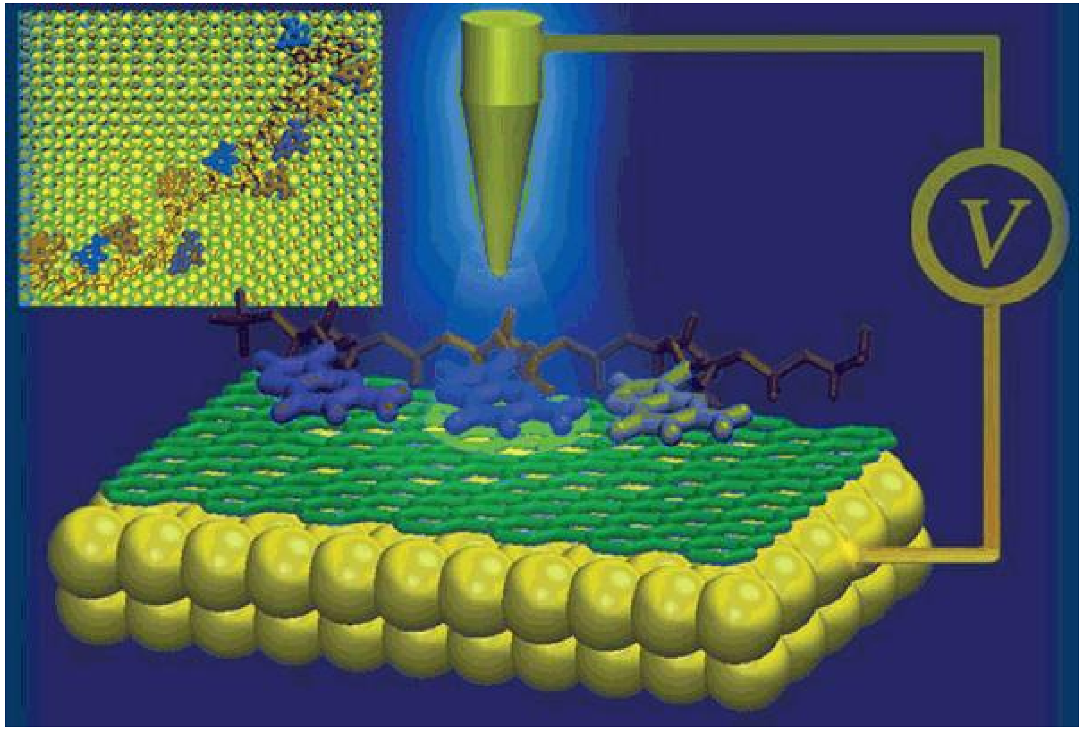
对于任意形状的势垒

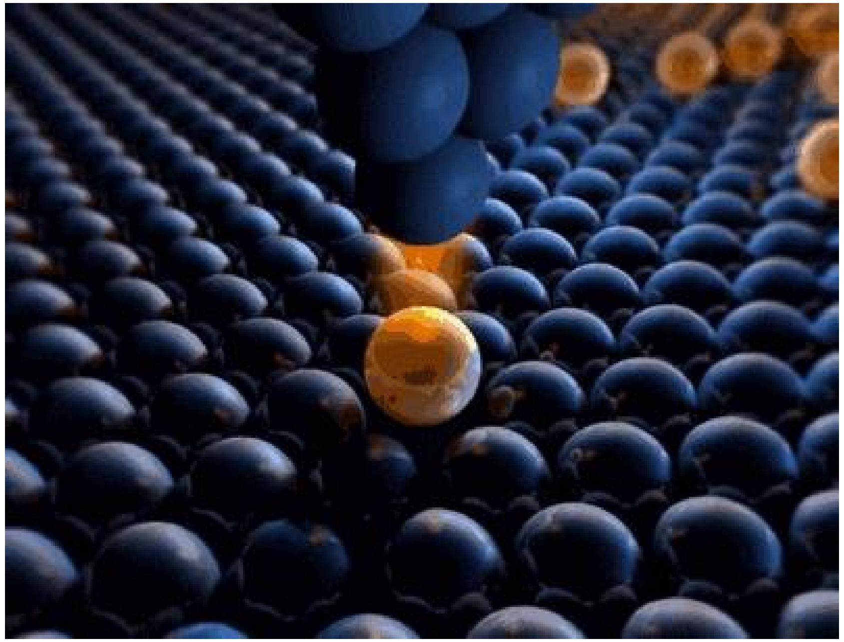
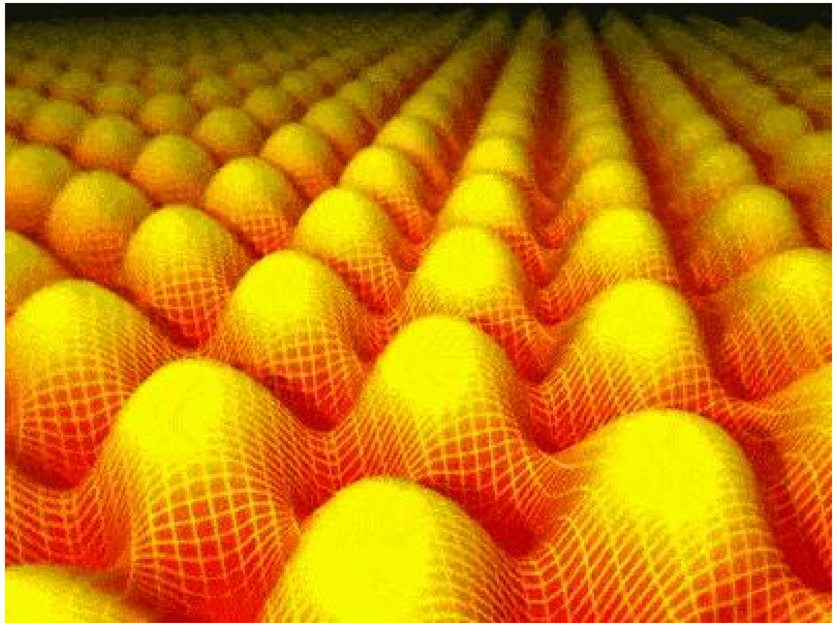
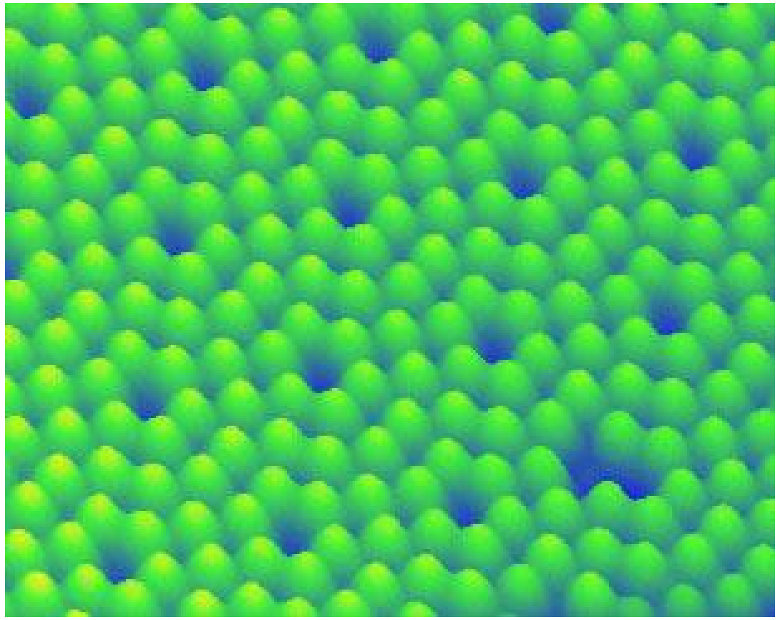
$$T_{\text{透射系数}} = T_0 e^{-\frac{2a}{\hbar}\int_{x_1}^{x_2}\sqrt{2m\left(U(x)-E\right)}dx}$$

●扫描隧穿显微镜（STM）

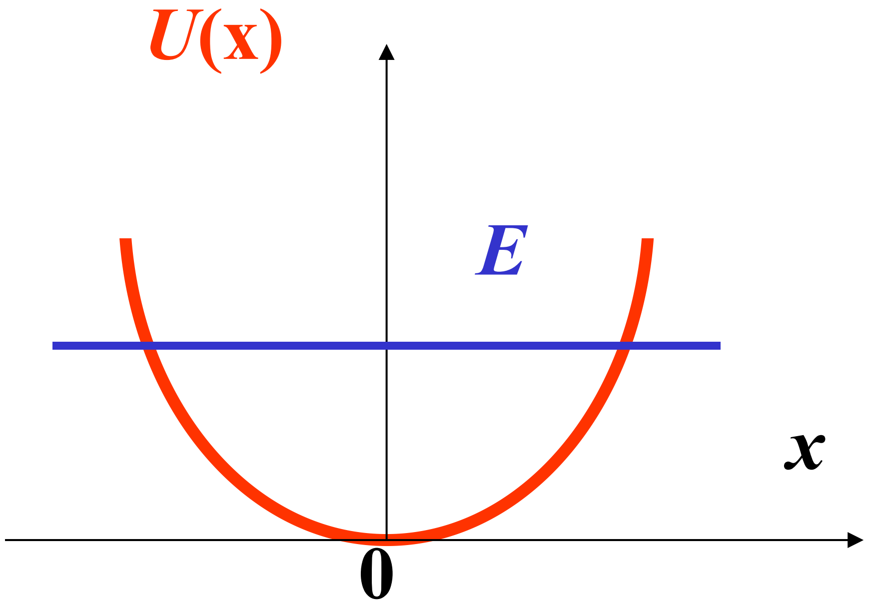
(Scanning Tunneling Microscope)
是观察固体表面原子情况的超高倍显微镜。

➢原理　隧道电流 i 与样品和针尖间的距离S关系极为敏感。



4.2 线性谐振子



4.2 线性谐振子

在经典力学中，当质量为 μ 的粒子，受弹性力F = - kx作用，由牛顿第二定律可以写出运动方程为：

$$\mu\frac{d^2x}{dt^2}=-kx\to x''+\omega^2x=0 \text{其中} \omega=\sqrt{\frac{k}{\mu}} \qquad \to U_{\text{势能}}=\frac{1}{2}kx^2=\frac{1}{2}\mu\omega^2x^2$$

线性谐振子的 Hamilton量：

$$\to\hat{H}_{\text{哈密顿算符}}=\frac{\hat{p}^2}{2\mu_{(\text{谐振子质量})}}+\frac{1}{2}\mu\omega^2x^2=-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}+\frac{1}{2}\mu\omega^2x^2$$

则Schrodinger 方程可写为 ：

$$\to\left\{\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}+[E-\frac{1}{2}\mu\omega^2x^2]\right\}\psi(x)=0$$

为简单计， 引入无量纲变量ξ代替x， 令：$\xi=\alpha x$ 其中 $\alpha=\sqrt{\frac{\mu\omega}{\hbar}}$,则方程可改写为:

$$\to\frac{d^2\psi(\xi)}{d\xi^2}+[\lambda-\xi^2]\psi(\xi)=0, \text{其中} \lambda=\frac{2E}{\hbar\omega}$$

$$\rightarrow \frac{d^2\psi(\xi)}{d\xi^2}+[\lambda-\xi^2]\psi(\xi)=0,\text{其中}\lambda=\frac{2E}{\hbar\omega}$$

1. 渐近解:为求解方程，我们先看一下它的渐近解，即当 ξ →±∞ 时波函数 ψ 的行为。在此情况下， λ << ξ 2，于是方程变为：

$$\rightarrow \frac{d^2\psi_\infty}{d\xi^2}-\xi^2\psi_\infty=0 \qquad \rightarrow \psi_\infty=C_1e^{-\frac{\xi^2}{2}}+C_2e^{\frac{\xi^2}{2}}$$

根据波函数有限条件，$C_2=0$，所以:$\rightarrow \psi_\infty=C_1e^{-\frac{\xi^2}{2}}$

求方程$\frac{d^2\psi}{d\xi^2}+[\lambda-\xi^2]\psi=0$的波函数$\psi$,在无穷远处有$\psi_\infty=e^{-\xi^2/2}$渐近形式，自然会令：

$$\psi(\xi)=H(\xi)e^{-\xi^2/2}$$

- 其中 H(ξ) 必须满足波函数的单值、有限、连续的标准条件。即：

① 当 ξ 有限时，H(ξ)有限；

② 当 ξ →∞时，H(ξ)的行为要保证 ψ(ξ)→ 0。

$$\psi(\xi)=H(\xi)e^{-\xi^2/2}\text{代入}\rightarrow\frac{d^2\psi}{d\xi^2}+[\lambda-\xi^2]\psi(x)=0$$

$$\rightarrow\frac{d^2H}{d\xi^2}-2\xi\frac{dH}{d\xi}+(\lambda-1)H=0$$

试探解：

1）如果$H(\xi)=\mathrm{a}_0$（常数），带入$\rightarrow\dfrac{d^2H}{d\xi^2}-2\xi\dfrac{dH}{d\xi}+(\lambda-1)H=0$

必然有$\rightarrow\lambda=1\rightarrow\lambda=\dfrac{2E}{\hbar\omega}\rightarrow E_{\text{本征能量}}=\dfrac{1}{2}\hbar\omega$

$H(\xi)=a_0\rightarrow$对应波函数$\psi(\xi)=a_0e^{-\xi^2/2}$

再根据定义$\xi=\alpha x$其中$\alpha=\sqrt{\dfrac{\mu\omega}{\hbar}}$,则波函数$\psi(x)=a_0e^{-\frac{\mu\omega}{2\hbar}x^2}$

$$归一化：\int_{-\infty}^{\infty}\left(\psi(x)\right)^2 dx=\int_{-\infty}^{\infty}a_0^2 e^{-\frac{\mu\omega}{\hbar}x^2}dx=1$$

$$同理：\int_{-\infty}^{\infty}\left(\psi(y)\right)^2 dy=\int_{-\infty}^{\infty}a_0^2 e^{-\frac{\mu\omega}{\hbar}y^2}dy=1$$

$$\rightarrow\int_{-\infty}^{\infty}a_0^2 e^{-\frac{\mu\omega}{\hbar}x^2}dx\int_{-\infty}^{\infty}a_0^2 e^{-\frac{\mu\omega}{\hbar}y^2}dy=a_0^4\int_0^{\infty}e^{-\frac{\mu\omega}{\hbar}r^2}rdr\int_0^{2\pi}d\theta=a_0^4\left(\frac{\hbar}{2\mu\omega}\right)2\pi=1$$

$$a_0^2=\sqrt{\frac{\mu\omega}{\hbar\pi}}\qquad a_0^2=\sqrt{\frac{\mu\omega}{\hbar\pi}}\rightarrow\psi_0(x)=\sqrt[4]{\frac{\mu\omega}{\hbar\pi}}e^{-\frac{\mu\omega}{2\hbar}x^2}$$

$$则E_{0本征能量}=\frac{1}{2}\hbar\omega\rightarrow\psi_0(x)=\sqrt[4]{\frac{\mu\omega}{\hbar\pi}}e^{-\frac{\mu\omega}{2\hbar}x^2}$$

2) 如果$H\left(\xi\right)=a_1\xi$，带入$\rightarrow\dfrac{d^2H}{d\xi^2}-2\xi\dfrac{dH}{d\xi}+(\lambda-1)H=0$

$\rightarrow -2\xi a_1+(\lambda-1)a_1\xi=0\rightarrow\lambda=3$ $\qquad\lambda=3\rightarrow\lambda=\dfrac{2E}{\hbar\omega}\rightarrow E_{本征能量}=\dfrac{3}{2}\hbar\omega$

$H\left(\xi\right)=a_1\xi\rightarrow$对应波函数$\psi(\xi)=a_1\xi e^{-\xi^2/2}$

再根据定义$\xi=\alpha x$其中$\alpha=\sqrt{\dfrac{\mu\omega}{\hbar}}$,则波函数$\psi(x)=a_1\alpha x e^{-\frac{\mu\omega}{2\hbar}x^2}$

$$\int_{-\infty}^{\infty}\left(\psi(\xi)\right)^2dx=\int_{-\infty}^{\infty}\left(a_1\alpha x\right)^2e^{-\frac{\mu\omega}{\hbar}x^2}dx=1$$

$$\rightarrow\left(a_1\alpha\right)^2\int_{-\infty}^{\infty}x^2e^{-\frac{\mu\omega}{\hbar}x^2}dx=\left(a_1\alpha\right)^2\left[\left(-\frac{\hbar}{2\mu\omega}\right)xd\left(e^{-\frac{\mu\omega}{\hbar}x^2}\right)\Bigg|_{-\infty}^{+\infty}+\frac{\hbar}{2\mu\omega}\int_{-\infty}^{\infty}e^{-\frac{\mu\omega}{\hbar}x^2}dx\right]=1$$

$$\rightarrow\left(a_1\alpha\right)^2\left[0+\frac{\hbar}{2\mu\omega}\int_{-\infty}^{\infty}e^{-\frac{\mu\omega}{\hbar}x^2}dx\right]=\left(a_1\alpha\right)^2\left[\frac{\hbar}{2\mu\omega}\int_{-\infty}^{\infty}e^{-\frac{\mu\omega}{\hbar}x^2}dx\right]=1$$

$$\int_{-\infty}^{\infty} e^{-\frac{\mu\omega}{\hbar}x^2}dx\int_{-\infty}^{\infty} e^{-\frac{\mu\omega}{\hbar}y^2}dy=\int_0^{\infty} e^{-\frac{\mu\omega}{\hbar}r^2}rdr\int_0^{2\pi}d\theta=2\pi\left(\frac{\hbar}{2\mu\omega}\right)=\frac{\pi\hbar}{\mu\omega}\quad\to\int_{-\infty}^{\infty} e^{-\frac{\mu\omega}{\hbar}x^2}=\sqrt{\frac{\pi\hbar}{\mu\omega}}$$

$$\int_{-\infty}^{\infty} e^{-\frac{\mu\omega}{\hbar}x^2}=\sqrt{\frac{\pi\hbar}{\mu\omega}}\to(a_1\alpha)^2\left[\frac{\hbar}{2\mu\omega}\int_{-\infty}^{\infty} e^{-\frac{\mu\omega}{\hbar}x^2}dx\right]=1\to(a_1\alpha)^2\left[\frac{\hbar}{2\mu\omega}\sqrt{\frac{\pi\hbar}{\mu\omega}}\right]=1$$

$$(a_1\alpha)^2\left[\frac{\hbar}{2\mu\omega}\sqrt{\frac{\pi\hbar}{\mu\omega}}\right]=1\to a_1\alpha=\sqrt{\frac{2\mu\omega}{\hbar}\sqrt{\frac{\mu\omega}{\pi\hbar}}}$$

$$a_1\alpha=\sqrt{\frac{2\mu\omega}{\hbar}\sqrt{\frac{\mu\omega}{\pi\hbar}}}\text{代入}\psi(x)=a_1\alpha x e^{-\frac{\mu\omega}{2\hbar}x^2}\to\psi_1(x)=\sqrt{\frac{2\mu\omega}{\hbar}\sqrt{\frac{\mu\omega}{\pi\hbar}}}xe^{-\frac{\mu\omega}{2\hbar}x^2}$$

$$E_1=\frac{3}{2}\hbar\omega\to\psi_1(x)=\sqrt{\frac{2\mu\omega}{\hbar}\sqrt{\frac{\mu\omega}{\pi\hbar}}}xe^{-\frac{\mu\omega}{2\hbar}x^2}$$

3) 如果$H(\xi)=a_0+a_2\xi^2$（常数），带入$\rightarrow \frac{d^2H}{d\xi^2}-2\xi\frac{dH}{d\xi}+(\lambda-1)H=0$

$$\rightarrow 2a_2-4\xi^2a_2+(\lambda-1)\left(a_0+a_2\xi^2\right)=0$$

$$\rightarrow \begin{cases} -4\xi^2a_2+(\lambda-1)a_2\xi^2=0 \\ 2a_2+(\lambda-1)a_0=0 \end{cases} \rightarrow \lambda=5, a_2=-2a_0 \qquad \lambda=5\rightarrow\lambda=\frac{2E}{\hbar\omega}\rightarrow E_2=\frac{5}{2}\hbar\omega$$

$\lambda=5, a_2=-2a_0$代入$\rightarrow H(\xi)=a_0+a_2\xi^2\rightarrow H(\xi)=a_0\left(1-2\xi^2\right)$

$$H(\xi)=a_0\left(1-2\xi^2\right)\rightarrow\psi(\xi)=a_0\left(1-2\xi^2\right)e^{-\xi^2/2}$$

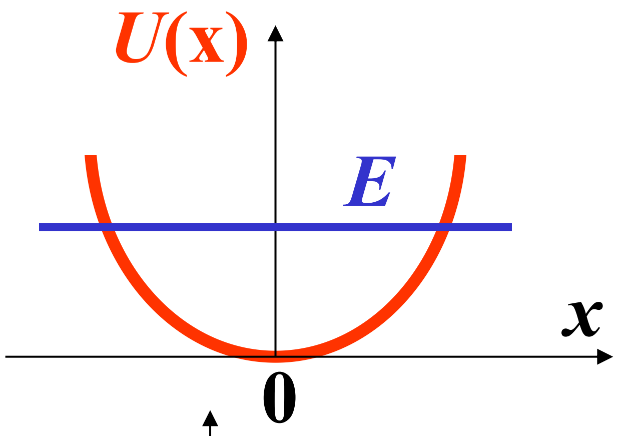
再根据定义$\xi=\alpha x$其中$\alpha=\sqrt{\frac{\mu\omega}{\hbar}}$,则波函数$\psi(x)=a_0\left(1-2\alpha x^2\right)e^{-\frac{\mu\omega}{2\hbar}x^2}$

利用归一化方法得到$\rightarrow\psi(x)=\sqrt{\frac{\mu\omega}{2\hbar\sqrt{\pi}}}\left(\frac{2\mu\omega}{\hbar}x^2-1\right)e^{-\frac{\mu\omega}{2\hbar}x^2}$

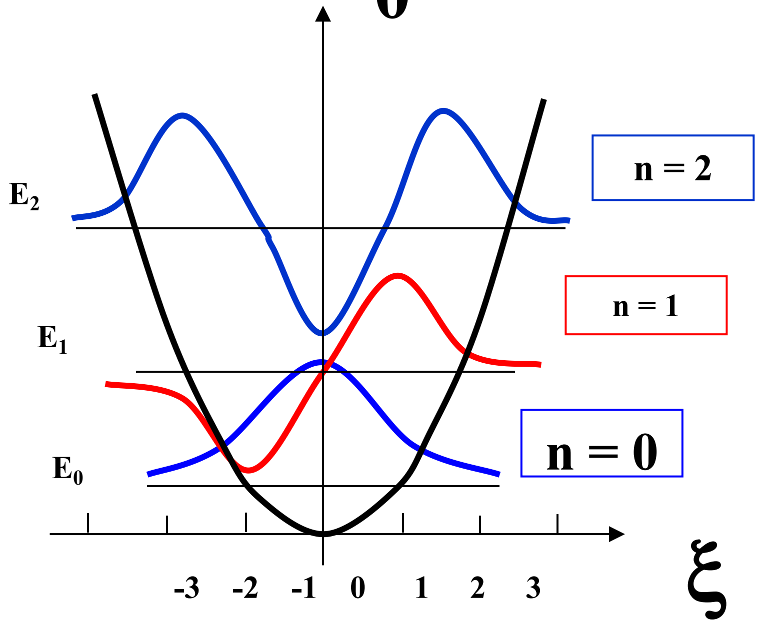
$$\mathrm{E}_2=\frac{5}{2}\hbar\omega\rightarrow\psi(x)=\sqrt{\frac{\mu\omega}{2\hbar\sqrt{\pi}}}\left(\frac{2\mu\omega}{\hbar}x^2-1\right)e^{-\frac{\mu\omega}{2\hbar}x^2}$$

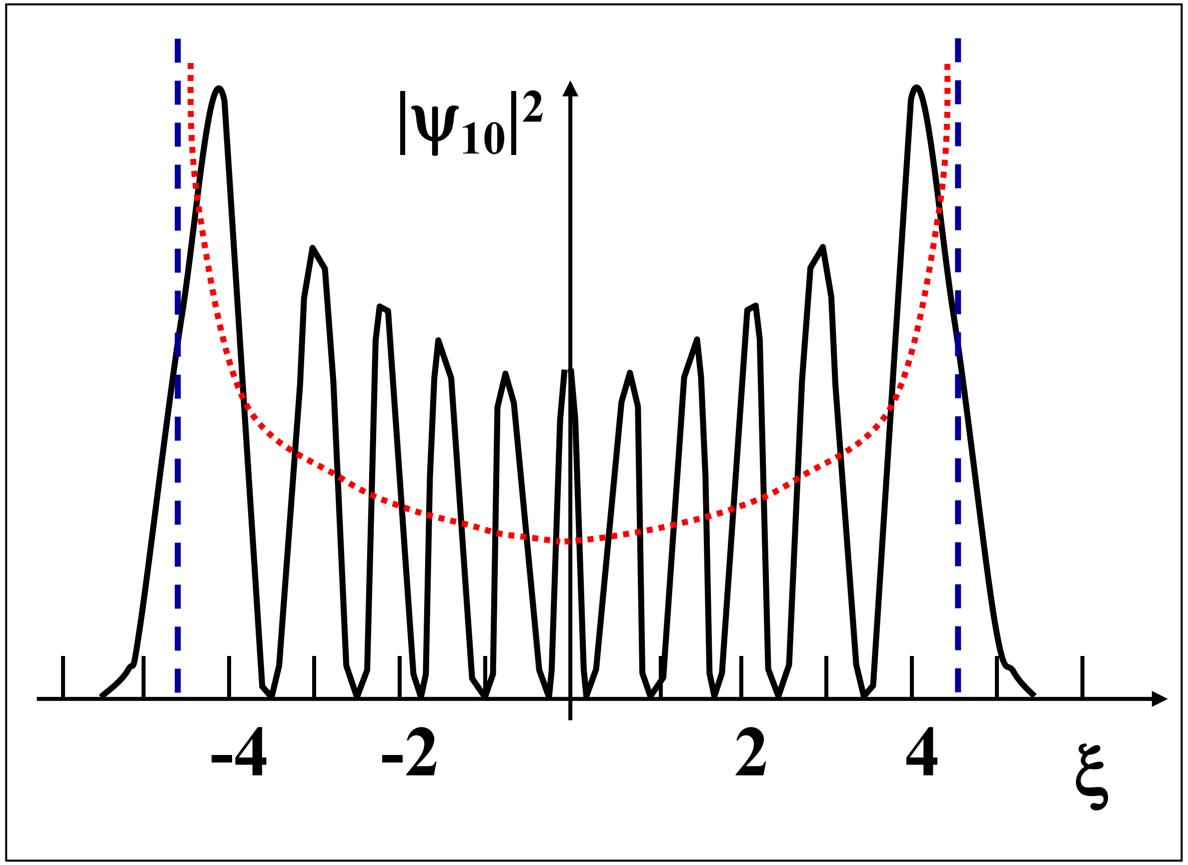
总结

$$\rightarrow \left\{ \frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + [E - \frac{1}{2}\mu\omega^2 x^2] \right\} \psi(x) = 0$$



$$\begin{cases} E_0 = \frac{1}{2}\hbar\omega \rightarrow \psi_0(x) = \sqrt[4]{\frac{\mu\omega}{\hbar\pi}} e^{-\frac{\mu\omega}{2\hbar}x^2} \\ E_1 = \frac{3}{2}\hbar\omega \rightarrow \psi_1(x) = \sqrt{\frac{2\mu\omega}{\hbar}} \sqrt{\frac{\mu\omega}{\pi\hbar}} x e^{-\frac{\mu\omega}{2\hbar}x^2} \\ E_2 = \frac{5}{2}\hbar\omega \rightarrow \psi(x) = \sqrt{\frac{\mu\omega}{2\hbar\sqrt{\pi}}} \left(\frac{2\mu\omega}{\hbar} x^2 - 1 \right) e^{-\frac{\mu\omega}{2\hbar}x^2} \\ E_n \ldots\ldots\ldots \end{cases}$$




$|\psi_{10}|^2$
-4
-2
2
4
ξ

例1．求三维谐振子能级，并讨论它的简并情况

解：（1）三维谐振子 Hamilton 量

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left[\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right]+\tfrac{1}{2}\mu\omega^2(x^2+y^2+z^2) = \hat{H}_x+\hat{H}_y+\hat{H}_z$$

$$\rightarrow\begin{cases}\hat{H}_x = -\dfrac{\hbar^2}{2\mu}\dfrac{d^2}{dx^2}+\tfrac{1}{2}\mu\omega^2x^2\\ \hat{H}_y = -\dfrac{\hbar^2}{2\mu}\dfrac{d^2}{dy^2}+\tfrac{1}{2}\mu\omega^2y^2\\ \hat{H}_z = -\dfrac{\hbar^2}{2\mu}\dfrac{d^2}{dz^2}+\tfrac{1}{2}\mu\omega^2z^2\end{cases}$$

$$\hat{H}\psi(x,y,z) = \left(\hat{H}_x+\hat{H}_y+\hat{H}_z\right)\psi(x,y,z) = E\psi(x,y,z)$$

$$\rightarrow\begin{cases}E_{n_1n_2n_3} = E_{n_1}+E_{n_1}+E_{n_1}\\ \psi_{n_1n_2n_3}(x,y,z) = \psi_{n_1}(x)\psi_{n_2}(y)\psi_{n_3}(z)\end{cases}$$

$$\hat{H}\psi\left(x,y,z\right)=\left(\hat{H}_x+\hat{H}_y+\hat{H}_z\right)\psi\left(x,y,z\right)=E\psi\left(x,y,z\right)$$

$$\begin{cases}\hat{H}=\hat{H}_x+\hat{H}_y+\hat{H}_z\\ E=E_1+E_2+E_3\\ \psi\left(x,y,z\right)=\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)\end{cases}\qquad \left(\hat{H}_x+\hat{H}_y+\hat{H}_z\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)=\left(E_1+E_2+E_3\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)$$

$$\rightarrow\begin{cases}\left(\hat{H}_x\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)=\left(E_1\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)\\ \left(\hat{H}_y\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)=\left(E_2\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)\\ \left(\hat{H}_z\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)=\left(E_3\right)\psi\left(x\right)\psi\left(y\right)\psi\left(z\right)\end{cases}\rightarrow\begin{cases}\hat{H}_x\psi\left(x\right)=E_1\psi\left(x\right)\\ \hat{H}_y\psi\left(y\right)=E_2\psi\left(y\right)\\ \hat{H}_z\psi\left(z\right)=E_3\psi\left(z\right)\end{cases}$$

$$\rightarrow\begin{cases}\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}+\frac{1}{2}\mu\omega^2x^2\right)\psi\left(x\right)=E_1\psi\left(x\right)\\ \left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dy^2}+\frac{1}{2}\mu\omega^2y^2\right)\psi\left(y\right)=E_2\psi\left(y\right)\\ \left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2}+\frac{1}{2}\mu\omega^2z^2\right)\psi\left(z\right)=E_3\psi\left(z\right)\end{cases}\qquad i=1,2,3\begin{cases}E_{i0}=\frac{1}{2}\hbar\omega\rightarrow\psi_0(x)=\sqrt[4]{\frac{\mu\omega}{\hbar\pi}}e^{-\frac{\mu\omega}{2\hbar}x^2}\\ E_{i1}=\frac{3}{2}\hbar\omega\rightarrow\psi_1(x)=\sqrt{\frac{2\mu\omega}{\hbar}\sqrt{\frac{\mu\omega}{\pi\hbar}}}xe^{-\frac{\mu\omega}{2\hbar}x^2}\\ E_{i2}=\frac{5}{2}\hbar\omega\rightarrow\psi(x)=\sqrt{\frac{\mu\omega}{2\hbar\sqrt{\pi}}}\left(\frac{2\mu\omega}{\hbar}x^2-1\right)e^{-\frac{\mu\omega}{2\hbar}x^2}\end{cases}$$

$$i=1,2,3\begin{cases}E_{i0}=\frac{1}{2}\hbar\omega\rightarrow\psi_0(x)=\sqrt[4]{\frac{\mu\omega}{\hbar\pi}}e^{-\frac{\mu\omega}{2\hbar}x^2}\\E_{i1}=\frac{3}{2}\hbar\omega\rightarrow\psi_1(x)=\sqrt{\frac{2\mu\omega}{\hbar}\sqrt{\frac{\mu\omega}{\pi\hbar}}}xe^{-\frac{\mu\omega}{2\hbar}x^2}\\E_{i2}=\frac{5}{2}\hbar\omega\rightarrow\psi(x)=\sqrt{\frac{\mu\omega}{2\hbar\sqrt{\pi}}}\left(\frac{2\mu\omega}{\hbar}x^2-1\right)e^{-\frac{\mu\omega}{2\hbar}x^2}\end{cases}$$

$$i=1,2,3\rightarrow\begin{cases}E_{n_1n_2n_3}=E_{n_1}+E_{n_2}+E_{n_3}\\\psi_{n_1n_2n_3}(x,y,z)=\psi_{n_1}(x)\psi_{n_2}(y)\psi_{n_3}(z)\end{cases}$$

$$E_N=(n_1+n_2+n_3+\tfrac{3}{2})\hbar\omega=(N+\tfrac{3}{2})\hbar\omega\text{其中}\qquad N=n_1+n_2+n_3$$

对给定N= n_1 + n_2 + n_3 的组合方式数列表分析如下：						
n_1	n_2				→	组合方式数
0	0,	1,	...,	N	→	N+1
1	0,	1,	...,	N-1	→	N
2	0,	1,	...,	N-2	→	N-1
...,	...,	...,	...,	...	→	...
N	0,				→	1
对给定N（N= n_1 + n_2 + n_3 ），{n_1 ，n_2，n_3 }的组合方式数						(1/2)(N+1)(N+2)

例2. 荷电 q 的谐振子，受到沿 x 向外电 ε 的作用，其势场为：$U(x)=\frac{1}{2}\mu\omega^2x^2-q\varepsilon x$

求能量本征值和本征函数。

解：Schrodinger方程：

$$\frac{d^2}{dx^2}\psi(x)+\frac{2\mu}{\hbar^2}[E-U(x)]\psi(x)=0$$

$$U(x)=\frac{1}{2}\mu\omega^2x^2-q\varepsilon x=\frac{1}{2}\mu\omega^2[x-\frac{q\varepsilon}{\mu\omega^2}]^2-\frac{q^2\varepsilon^2}{2\mu\omega^2}=\frac{1}{2}\mu\omega^2(x-x_0)^2-U_0$$

其中：$x_0=\frac{q\varepsilon}{\mu\omega^2}$ $U_0=\frac{q^2\varepsilon^2}{2\mu\omega^2}$

$$\text{坐标变换}\rightarrow\begin{cases}x'=x-x_0\\ \hat{p}=-i\hbar\frac{d}{dx}=-i\hbar\frac{d}{dx'}=\hat{p}'\end{cases}$$

$$\rightarrow\hat{H}=\frac{\hat{p}^2}{2\mu}+\tfrac{1}{2}\mu\omega^2(x-x_0)^2-U_0$$

$$=\frac{\hat{p}'^2}{2\mu}+\tfrac{1}{2}\mu\omega^2x'^2-U_0$$

$$\hat{H}=\frac{\hat{p}'^2}{2\mu}+\tfrac{1}{2}\mu\omega^2x'^2-U_0 \rightarrow \frac{d^2\psi(x')}{dx'^2}+\frac{2\mu}{\hbar^2}[E-\tfrac{1}{2}\mu\omega^2x'^2+U_0]\psi(x')=0$$

令$E'=E+U_0 \rightarrow \dfrac{d^2}{dx'^2}\psi(x')+\dfrac{2\mu}{\hbar^2}[E'-\tfrac{1}{2}\mu\omega^2x'^2]\psi(x')=0$

$$\begin{cases} E_0'=\dfrac{1}{2}\hbar\omega \rightarrow \psi_0(x')=\sqrt[4]{\dfrac{\mu\omega}{\hbar\pi}}e^{-\frac{\mu\omega}{2\hbar}x'^2} \\ E_1'=\dfrac{3}{2}\hbar\omega \rightarrow \psi_1(x')=\sqrt{\dfrac{2\mu\omega}{\hbar}\sqrt{\dfrac{\mu\omega}{\pi\hbar}}}xe^{-\frac{\mu\omega}{2\hbar}x'^2} \\ E_2'=\dfrac{5}{2}\hbar\omega \rightarrow \psi(x')=\sqrt{\dfrac{\mu\omega}{2\hbar\sqrt{\pi}}}\left(\dfrac{2\mu\omega}{\hbar}x^2-1\right)e^{-\frac{\mu\omega}{2\hbar}x'^2} \end{cases}$$

$$\begin{cases} x'=x-x_0=x-\dfrac{q\varepsilon}{\mu\omega^2} \\ E=E'-U_0=E'-\dfrac{q^2\varepsilon^2}{2\mu\omega^2} \end{cases}$$