第 4 章 薛定谔方程与定态波函数

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 $\rightarrow\frac{\partial\psi(x,t)}{\partial t}=\psi(x)\frac{\partial f(t)}{\partial t}$

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

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

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

- 一个是变量为t 的方程

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

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

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

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

同时可以知道，在定态的条件下波函数与时间t无关

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

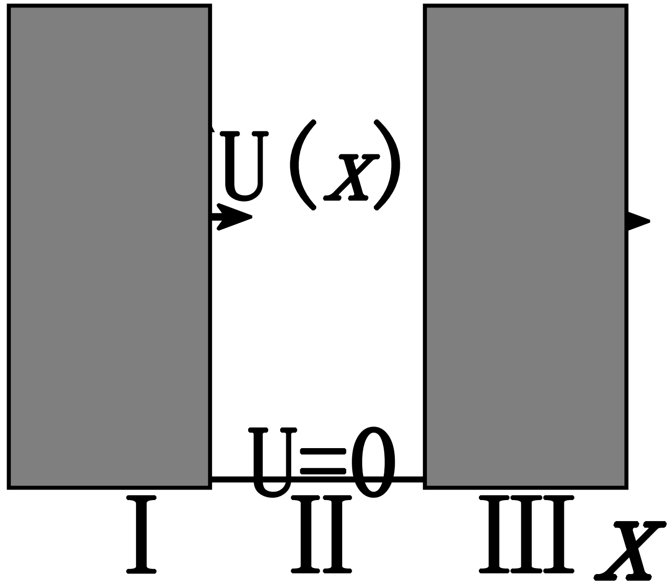
即定态时，概率密度可以用|(x)|²来表示，(x)称为定态波函数，

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：

它的势能函数为

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



无限深方势阱

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。

注意边界条件！

由于II区的 U(x)= 0，因此该区薛定谔方程为

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

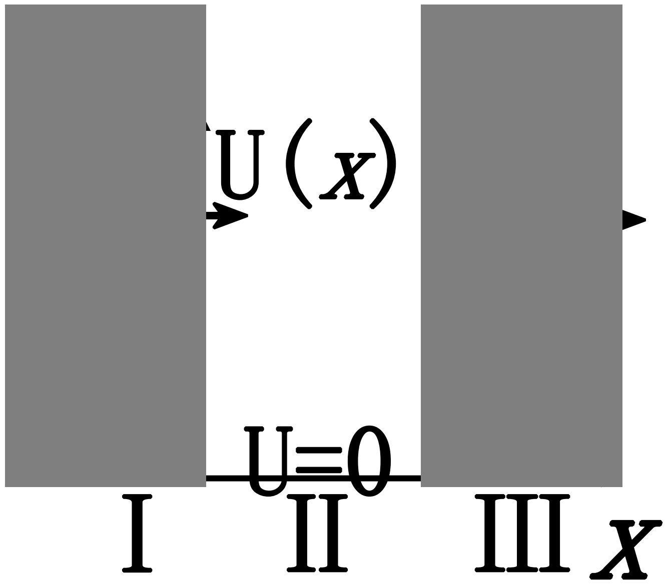
$$U=0\rightarrow-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}=E\psi(x)$$

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

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

$\psi(x)$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

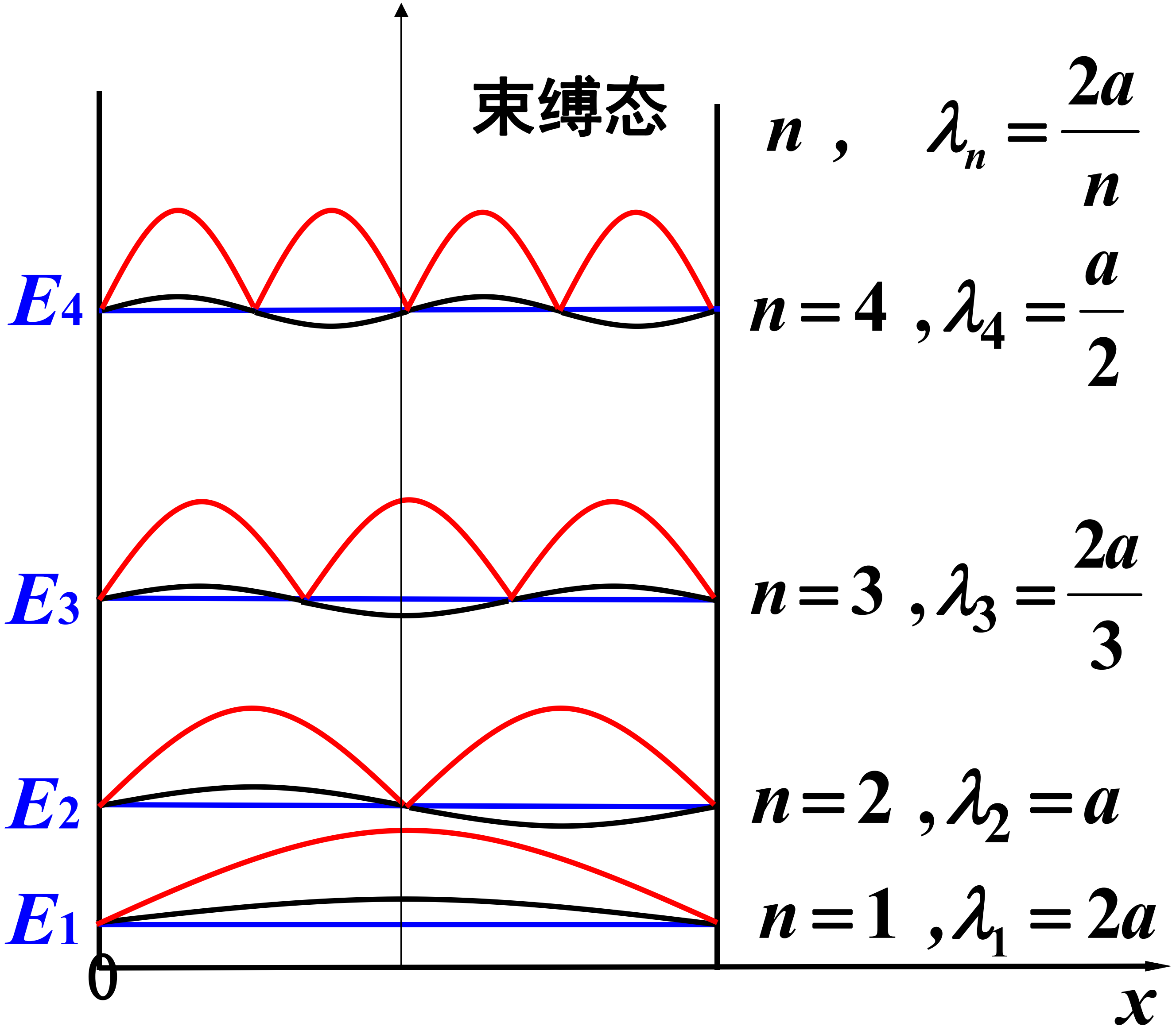
归一化条件 $\rightarrow \int_0^{2a} (\psi_o)^2 dx = \int_0^{2a} \left(A \sin \frac{n\pi}{a} x \right)^2 = 1 \qquad A = \sqrt{\frac{2}{a}}$

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

此处的k^2就相当于波中的波矢2π / λ

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

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。



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

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

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

$n=2\ ,\lambda_2 = a$

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

注意，由于波函数的周期性，其波的形状应该是个驻波。

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?

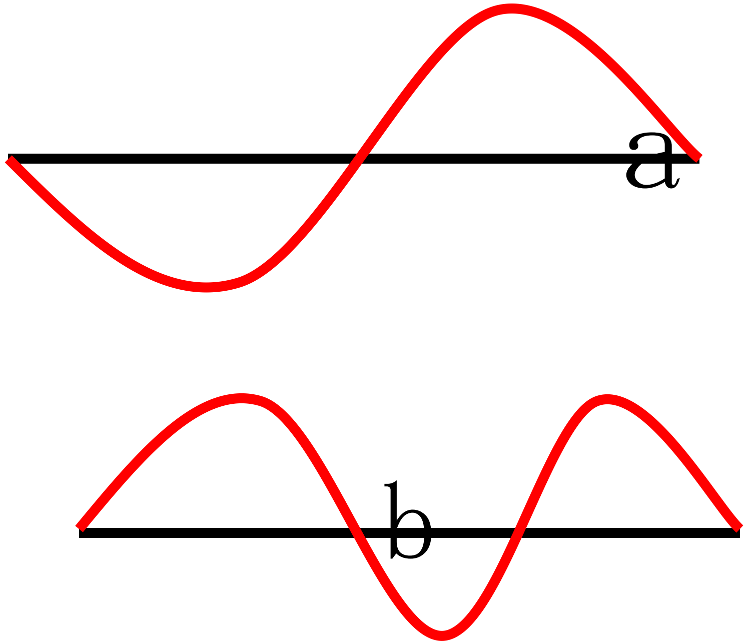
解:

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

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

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

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



例题2：计算微观粒子出现概率最大的位置？

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

解：

1）概率分布函数 $$F(x,t)=\psi^*(x,t)_n\,\psi(x,t)_n=\frac{2}{L}\cos^2\left(\frac{n\pi x}{L}\right)$$

2）最大概率位置

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

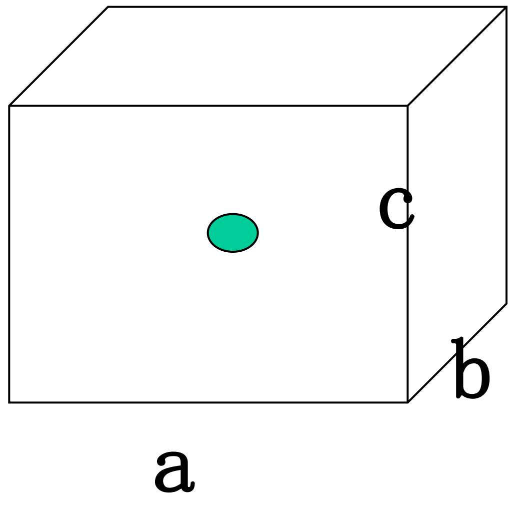
$$\left|\frac{4}{L}\frac{n\pi}{L}\cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)\right|=\left|\frac{2n\pi}{L^2}\sin\left(\frac{2n\pi x}{L}\right)\right|=0 \qquad x=0,\frac{L}{2},L$$

2. 三维无限深方势阱

三维无限深方势阱（考虑一个粒子被囚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 $\rightarrow \boldsymbol{\psi(x,y,z)=\psi(x)\psi(y)\psi(z)}$

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

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

有：$k^2=\frac{2m}{\hbar^2}E$

对于这种指数形式的相加，可以通过转化为独立变量相乘的方式来进行降维分别处理。

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

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

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

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

由此可以知道，一个粒子在三维空间中出现的概率与所处空间的尺寸有关。

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

类似三维矢量的叠加，可以理解为三维空间各个方向的波矢量的对应波矢的叠加

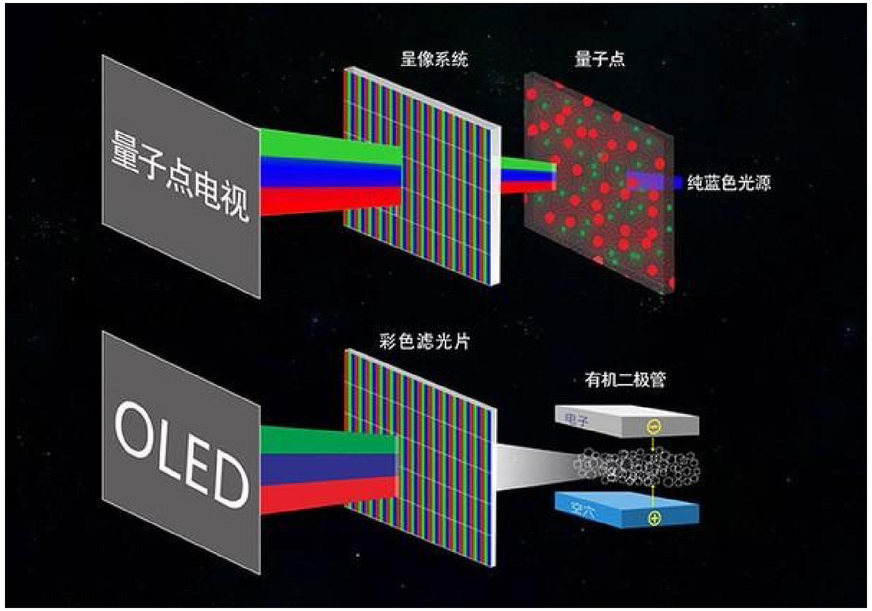
$$\text{利用} \rightarrow \begin{cases} \psi(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x, & k_x = \frac{n\pi}{a} \\ \psi(y) = \sqrt{\frac{2}{b}}\sin\frac{m\pi}{b}y & k_y = \frac{m\pi}{b} \\ \psi(z) = \sqrt{\frac{2}{c}}\sin\frac{l\pi}{c}z & k_z = \frac{l\pi}{c} \end{cases}$$

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

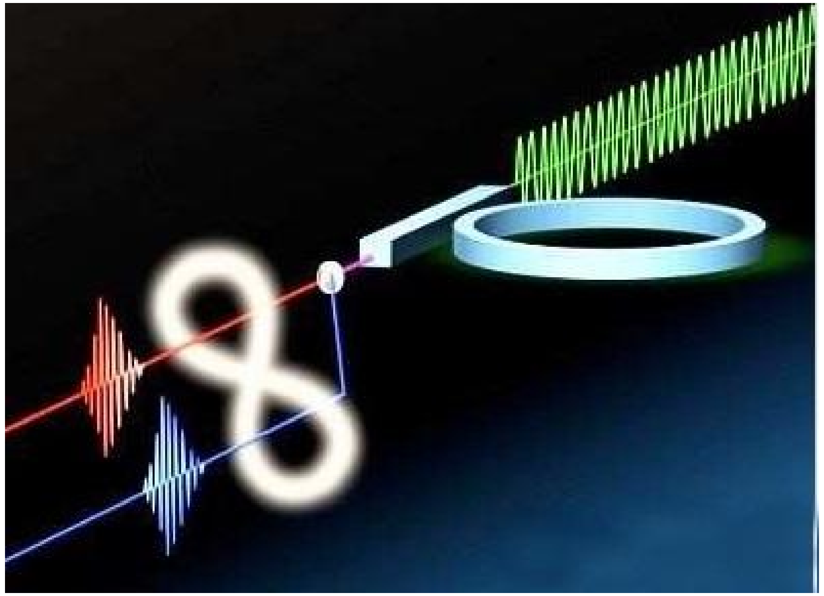
量子点的典型应用

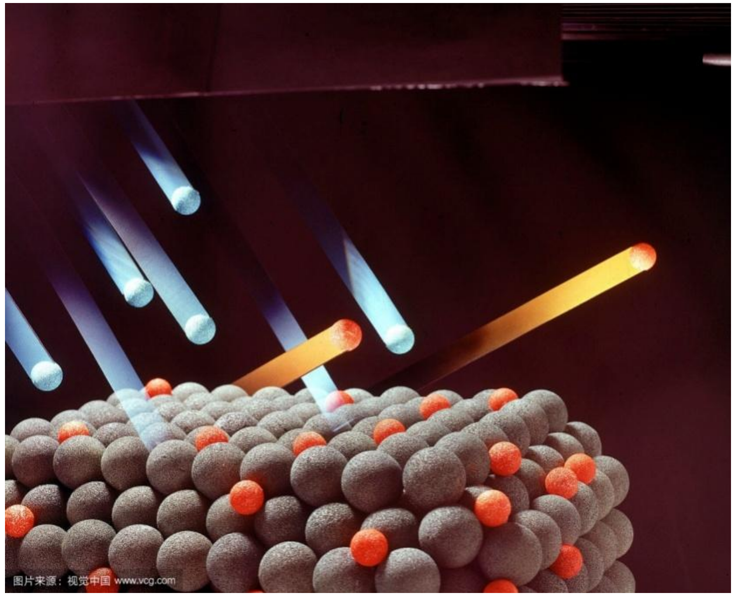
$$E_{\mathrm{n,m,l}} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \left(\frac{m\pi}{b}\right)^2 + \left(\frac{l\pi}{c}\right)^2\right] \qquad (n, l, m = 1, 2, 3, \ldots)$$

量子点电视

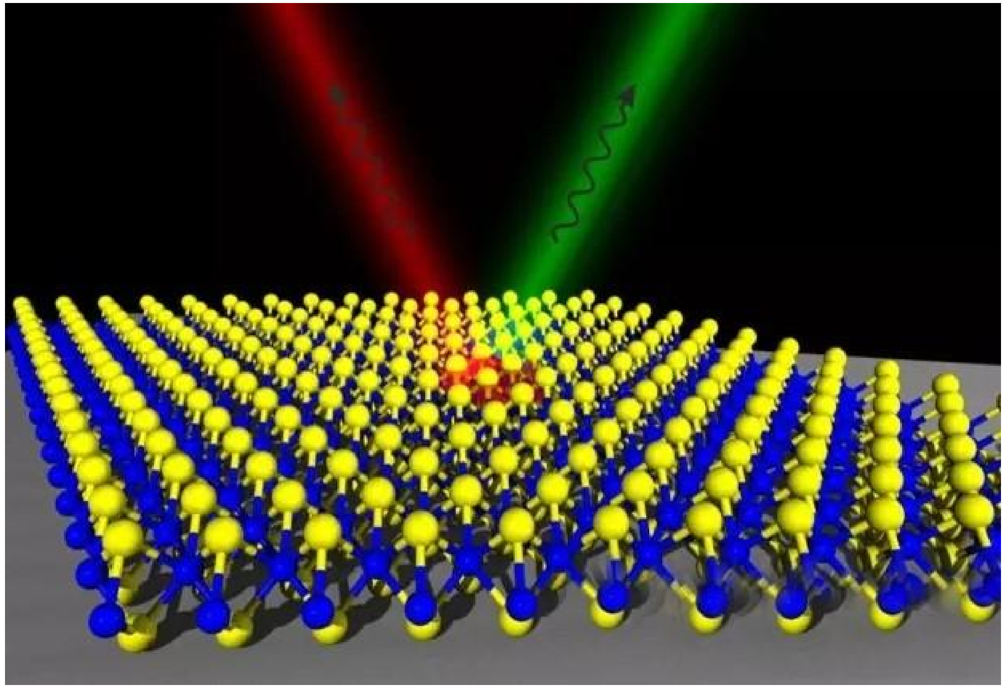


光子的分离





新型二维材料



3. 一维有限深方势阱（一）

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

U>E恒成立

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

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

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

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

可以直接省去两项的原因：波函数的平方描述的是自由粒子出现在某个位置的概率，并且概率一定是一个有限数值，故波函数中不能出现无穷项。

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

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

函数连续，导数不一定连续？？？

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

由于波函数有固定的周期，故其函数应该是驻波的形式，同时可以得出，A1 = A2

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

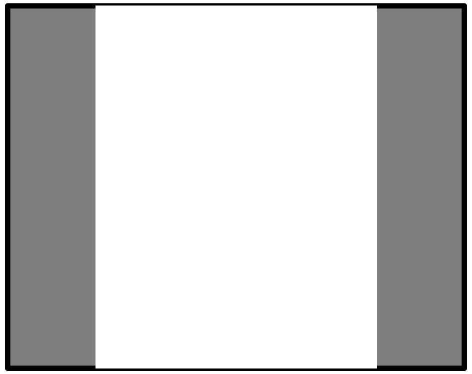
$$\begin{bmatrix} x = -a \\ x = a \end{bmatrix} \to \begin{cases} \psi'(-a) = A_1 \beta e^{-\beta a} \\ \psi'(-a) = i\alpha A_0 e^{-ia\alpha} - i\alpha B_0 e^{ia\alpha} \\ \psi'(a) = i\alpha A_0 e^{i\alpha a} - i\alpha B_0 e^{-i\alpha a} \\ \psi'(a) = -\beta A_2 e^{-\beta a} \end{cases} \to \begin{cases}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

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

$$\to \tan \alpha a = \pm \frac{\beta}{a}$$

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

3. 一维有限深方势阱（二）



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

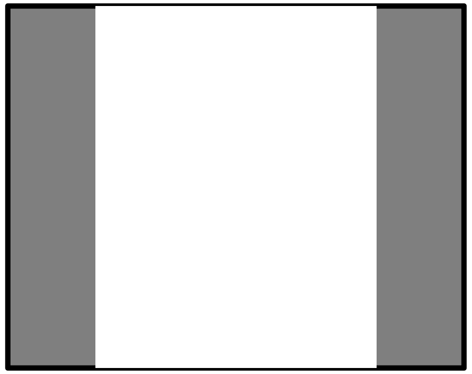
$$\tan\alpha a = \frac{-\left(\alpha^2-\beta^2\right) \pm \sqrt{\left(\alpha^2-\beta^2\right)^2 + 4\alpha^2\beta^2}}{2\alpha\beta} = \frac{\beta}{\alpha}$$

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

$$能量本征值 \rightarrow 2\alpha a = n\pi + \arctan\frac{\beta}{\alpha}$$

$$能量本征值 \rightarrow \sqrt{\frac{2m_0}{\hbar^2}E_x}\,a = n\pi + \arctan\frac{\beta}{\alpha}$$

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



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

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

4. 一维周期性有限深方势阱（二）

(了解为主)

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

$$\begin{cases}\alpha=\sqrt{\dfrac{2m}{\hbar^2}E}\\ \beta=\sqrt{\dfrac{2m}{\hbar^2}(E-U_0)}\\ \beta_0=\sqrt{\dfrac{2m}{\hbar^2}(U_1-E)},\end{cases}\rightarrow\begin{cases}\psi(x)=F_0e^{\beta_0 x} & U=U_1 & x\le 0\\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x} & U=0 & 0\le x\le b\\ \psi(x)=C_0e^{i\beta x}+D_0e^{-i\beta x} & U=U_0 & b\le x\le 2b\\ \psi(x)=A_1e^{i\alpha x}+B_1e^{-i\alpha x} & U=0 & 2b\le x\le 3b\\ \psi(x)=A_Ne^{-\beta_0(x-2Nb)} & U=U_1 & x\ge 2Nb\end{cases}$$

$$0\le x\le b\rightarrow\begin{cases}\psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x}\\ \psi'(x)=i\alpha A_0e^{i\alpha x}-i\alpha B_0e^{-i\alpha x}\end{cases}\ x=0\rightarrow\begin{cases}\psi(0)=A_0+B_0\\ \psi'(0)=i\alpha A_0-i\alpha B_0\end{cases}\quad \begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\begin{bmatrix}1 & 1\\ i\alpha & -i\alpha\end{bmatrix}\begin{bmatrix}A_0\\ B_0\end{bmatrix}$$

$$x=b\rightarrow\begin{cases}\psi(b)=A_0e^{i\alpha b}+B_0e^{-i\alpha b}\\ \psi'(b)=i\alpha A_0e^{i\alpha b}-i\alpha B_0e^{-i\alpha b}\end{cases}\rightarrow\begin{cases}A_0=\dfrac{i\alpha\psi(b)+\psi'(b)}{2i\alpha}e^{-i\alpha b}\\ B_0=\dfrac{i\alpha\psi(b)-\psi'(b)}{2i\alpha}e^{i\alpha b}\end{cases}$$

$$\rightarrow\begin{bmatrix}A_0\\B_0\end{bmatrix}=\frac{1}{2i\alpha}\begin{bmatrix}i\alpha e^{-i\alpha b} & e^{-i\alpha b}\\ i\alpha e^{i\alpha b} & -e^{i\alpha b}\end{bmatrix}\begin{bmatrix}\psi(b)\\ \psi'(b)\end{bmatrix}\qquad\rightarrow\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\begin{bmatrix}1 & 1\\ i\alpha & -i\alpha\end{bmatrix}\begin{bmatrix}A_0\\B_0\end{bmatrix}$$

$$\rightarrow\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\frac{1}{2i\alpha}\begin{bmatrix}1 & 1\\ i\alpha & -i\alpha\end{bmatrix}\begin{bmatrix}i\alpha e^{-i\alpha b} & e^{-i\alpha b}\\ i\alpha e^{i\alpha b} & -e^{i\alpha b}\end{bmatrix}\begin{bmatrix}\psi(b)\\ \psi'(b)\end{bmatrix}\qquad\rightarrow\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\begin{bmatrix}\cos\alpha b & -\dfrac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}\psi(b)\\ \psi'(b)\end{bmatrix}$$

相同的处理方法 $\rightarrow\begin{bmatrix}\psi(b)\\ \psi'(b)\end{bmatrix}=\begin{bmatrix}\cos\beta b & -\dfrac{1}{\beta}\sin\beta b\\ \beta\sin\beta b & \cos\beta b\end{bmatrix}\begin{bmatrix}\psi(b+b)\\ \psi'(b+b)\end{bmatrix}$

$$\rightarrow\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\begin{bmatrix}\cos\alpha b & -\dfrac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}\cos\beta b & -\dfrac{1}{\beta}\sin\beta b\\ \beta\sin\beta b & \cos\beta b\end{bmatrix}\begin{bmatrix}\psi(b+b)\\ \psi'(b+b)\end{bmatrix}$$

$$\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\begin{pmatrix}\cos\alpha b\cos\beta b-\frac{\beta}{\alpha}\sin\alpha b\sin\beta b & -\frac{1}{\beta}\cos\alpha b\sin\beta b-\frac{1}{\alpha}\sin\alpha b\cos\beta b\\ \alpha\sin\alpha b\cos\beta b+\beta\cos\alpha b\sin\beta b & -\frac{\alpha}{\beta}\sin\alpha b\sin\beta b+\cos\alpha b\cos\beta b\end{pmatrix}^N\begin{bmatrix}\psi\left(N\left(b_1+b_2\right)\right)\\ \psi'\left(N\left(b_1+b_2\right)\right)\end{bmatrix}$$

$$\begin{cases}m_{11}=\cos\alpha b\cos\beta b-\frac{\beta}{\alpha}\sin\alpha b\sin\beta b,\\ m_{12}=-\frac{1}{\beta}\cos\alpha b\sin\beta b-\frac{1}{\alpha}\sin\alpha b\cos\beta b\\ m_{21}=\alpha\sin\alpha b\cos\beta b+\beta\cos\alpha b\sin\beta b\\ m_{22}=-\frac{\alpha}{\beta}\sin\alpha b\sin\beta b+\cos\alpha b\cos\beta b\end{cases}\rightarrow M^N=\begin{bmatrix}\cos\alpha b\cos\beta b-\frac{\beta}{\alpha}\sin\alpha b\sin\beta b & -\frac{1}{\beta}\cos\alpha b\sin\beta b-\frac{1}{\alpha}\sin\alpha b\cos\beta b\\ \alpha\sin\alpha b\cos\beta b+\beta\cos\alpha b\sin\beta b & -\frac{\alpha}{\beta}\sin\alpha b\sin\beta b+\cos\alpha b\cos\beta b\end{bmatrix}^N=\begin{bmatrix}m_{11} & m_{12}\\ m_{21} & m_{22}\end{bmatrix}^N$$

$$M^N=\begin{bmatrix}m_{11} & m_{12}\\ m_{21} & m_{22}\end{bmatrix}^N=\begin{bmatrix}m_{11}U_{N-1}(\chi)-U_{N-2}(\chi) & m_{12}U_{N-1}(\chi)\\ m_{21}U_{N-1}(\chi) & m_{22}U_{N-1}(\chi)-U_{N-2}(\chi)\end{bmatrix}$$

$$\begin{cases}U_N(\chi)=\dfrac{\sin\left(N+1\right)\arccos\chi}{\sqrt{1-\chi^2}}\\ \chi=\dfrac{1}{2}\left(m_{11}+m_{22}\right)=\dfrac{1}{2}\left(\left(\cos\alpha b\cos\beta b-\dfrac{\beta}{\alpha}\sin\alpha b\sin\beta b\right)+\left(-\dfrac{\alpha}{\beta}\sin\alpha b\sin\beta b+\cos\alpha b\cos\beta b\right)\right)\end{cases}$$

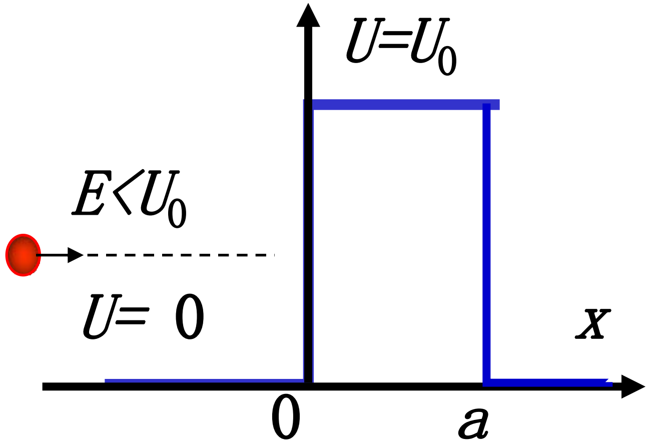
$$\begin{bmatrix} \psi(0) \\ \psi'(0) \end{bmatrix} = \begin{bmatrix} m_{11}U_{N-1}(\chi) - U_{N-2}(\chi) & m_{12}U_{N-1}(\chi) \\ m_{21}U_{N-1}(\chi) & m_{22}U_{N-1}(\chi) - U_{N-2}(\chi) \end{bmatrix} \begin{bmatrix} \psi\left(N\left(b_1 + b_2\right)\right) \\ \psi'\left(N\left(b_1 + b_2\right)\right) \end{bmatrix}$$

$$\begin{cases} U_N(\chi) = \dfrac{\sin\left(N+1\right)\arccos\chi}{\sqrt{1-\chi^2}} \\ \chi = \dfrac{1}{2}\left(m_{11} + m_{22}\right) = \dfrac{1}{2}\left(\left(\cos\alpha b\cos\beta b - \dfrac{\beta}{\alpha}\sin\alpha b\sin\beta b\right) + \left(-\dfrac{\alpha}{\beta}\sin\alpha b\sin\beta b + \cos\alpha b\cos\beta b\right)\right) \end{cases}$$

5. 隧道效应（势垒贯穿）

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：

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

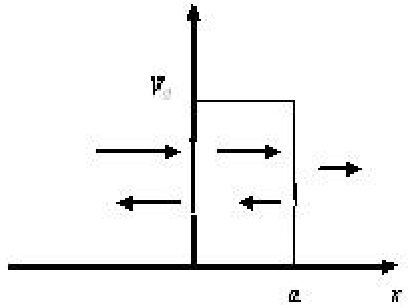
$$U(x)=\begin{cases}U_0, & 0<x<a\\ 0, & x<0, x>a\end{cases}$$

$$\begin{cases}\psi_1''+k_1^2\psi_1=0 & x<0 & I\ 区\\ \psi_2''+k_2^2\psi_2=0 & 0<x<a & II\ 区\\ \psi_3''+k_1^2\psi_3=0 & x>a & III\ 区\end{cases} \rightarrow \begin{cases}\psi_1(x)=Ae^{+ikx}+Be^{-ikx}\\ \psi_2(x)=De^{-k'x}+Fe^{+k'x} \qquad 0\le x\le a\\ \psi_3(x)=Ce^{+ikx}\end{cases} \leftarrow \begin{cases}k=\sqrt{\dfrac{2mE}{\hbar^2}}\\ k'=\sqrt{\dfrac{2m(U_0-E)}{\hbar^2}}\end{cases}$$

利用波函数的有限性来省略一些参数

●确定系数

利用波函数及微商连续条件



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

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

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

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

解方程组得：

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

4. 透射系数和反射系数

透射系数： 透射波几率流密度与入射波几率流密度之比称为透射系数$D = J_D/J_I$ 其物理意义是：描述贯穿到 $x > a$ 的 III区中的粒子在单位时间内流过垂直 x方向的单位面积的数目与入射粒子（在 $x < 0$ 的 I 区）在单位时间内流过垂直于x方向单位面积的数目之比。

II 反射系数：反射波几率流密度与入射波几率流密度之比称为反射系数 $R = J_R/J_I$

几率流密度矢量： $\vec{J}=\frac{i\hbar}{2\mu}[\psi\nabla\psi^{*}-\psi^{*}\nabla\psi]$

$$\vec{J}=\frac{i\hbar}{2\mu}[\psi\frac{d}{dx}\psi^{*}-\psi^{*}\frac{d}{dx}\psi]$$

则入射波几率流密度

$$J_{I}=\frac{i\hbar}{2\mu}[Ae^{ik_1x}\frac{d}{dx}A^{*}e^{-ik_1x}-A^{*}e^{-ik_1x}\frac{d}{dx}Ae^{ik_1x}=\frac{k_1\hbar}{\mu}|A|^{2}$$

反射波 ψ= A’exp[-ik₁x]，所以反射波几率流密度： $J_{R}=-\frac{k_1\hbar}{\mu}|B|^{2}$

对透射波 ψ= Cexp[ik₁x]，所以透射波几率流密度： $J_{D}=\frac{k_1\hbar}{\mu}|C|^{2}$

$$C=\frac{4k_1k_2e^{-ik_1a}}{(k_1+k_2)^2e^{-ik_2a}-(k_1-k_2)^2e^{ik_2a}}A \qquad B=\frac{2i(k_1^2-k_2^2)\sin k_2a}{(k_1+k_2)^2e^{-ik_2a}-(k_1-k_2)^2e^{ik_2a}}A$$

于是透射系数为:

$$D=\frac{J_D}{J_I}=\frac{|C|^2}{|A|^2}=\frac{4k_1^2k_2^2}{(k_1^2-k_2^2)^2\sin^2 k_2a+4k_1^2k_2^2}$$

同理得反射系数:

$$R=\frac{J_R}{J_I}=\frac{|B|^2}{|A|^2}=\frac{(k_1^2-k_2^2)^2\sin^2 k_2a}{(k_1^2-k_2^2)^2\sin^2 k_2a+4k_1^2k_2^2}$$

由以上二式显然有 D+R=1，说明入射粒子一部分贯穿势垒到 x > a 的III区，另一部分则被势垒反射回来。

例1：入射粒子为电子。

设 $E=1eV$，$V_0 = 2eV$，
$a = 2\times 10^{-8}$ cm = 2Å，
算得 $D \approx 0.51$。

若$a=5\times 10^{-8}$cm = 5 Å，
则 $D \approx 0.024$，可见
透射系数迅速减小。

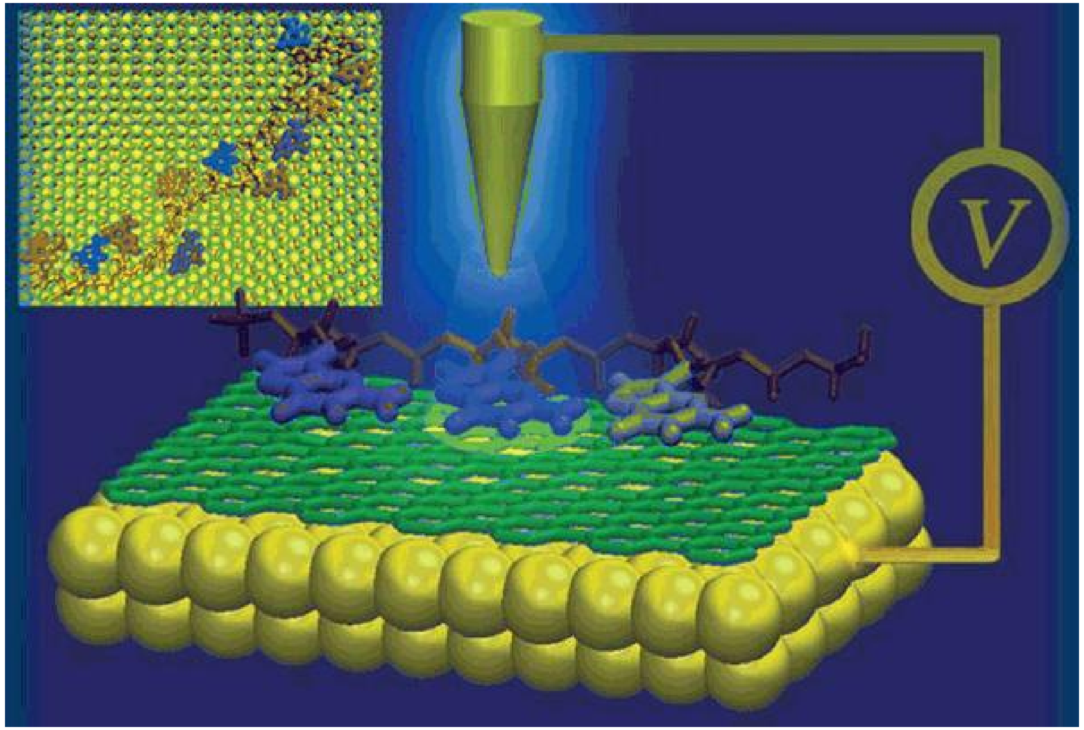
例2：入射粒子换成质子。

质子与电子质量比
$\mu_p/\mu_e \approx 1840$。
对于a = 2 Å
则 $D \approx 2 \times 10^{-38}$。
可见透射系数明显的依赖于
粒子的质量和势垒的宽度。

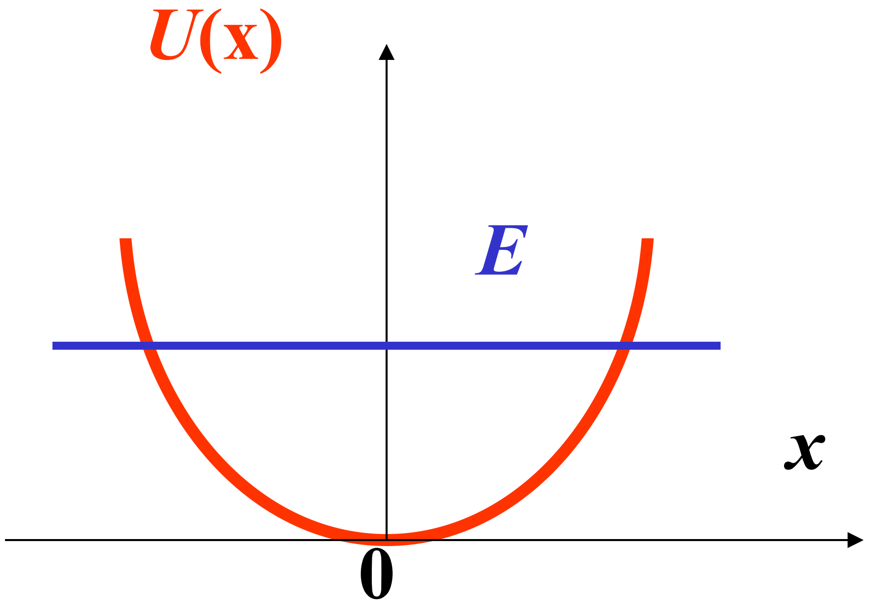
●扫描隧穿显微镜（STM）

(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：

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

线性谐振子的 Hamilton量： $\rightarrow\hat{H}_{\text{哈密顿算符}}=\dfrac{\hat{p}^2}{2\mu_{(\text{谐振子质量})}}+\dfrac{1}{2}\mu\omega^2x^2=-\dfrac{\hbar^2}{2\mu}\dfrac{d^2}{dx^2}+\dfrac{1}{2}\mu\omega^2x^2$

则Schrodinger 方程可写为 ：

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

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

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

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

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

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

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

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

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

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

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

$H(\xi)=a_1\xi\rightarrow$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$\psi(x)=a_1\alpha x e^{-\frac{\mu\omega}{2\hbar}x^2}$

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

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

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

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

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

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

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

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

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

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

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

$\lambda=5,a_2=-2a_0$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$\alpha=\sqrt{\dfrac{\mu\omega}{\hbar}}$,则波函数$\psi(x)=a_0\left(1-2\alpha x^2\right)e^{-\frac{\mu\omega}{2\hbar}x^2}$

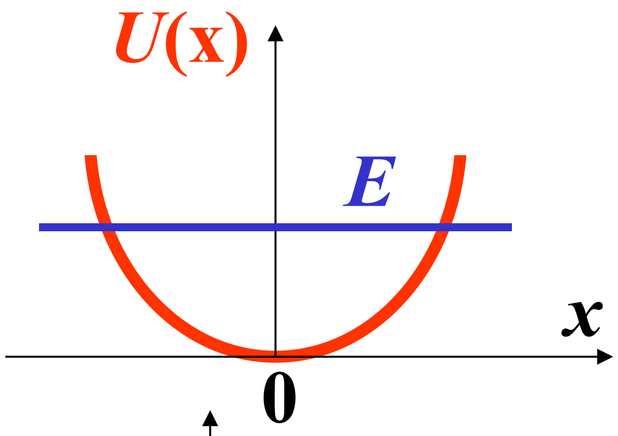
利用归一化方法得到$\rightarrow\psi(x)=\sqrt{\dfrac{\mu\omega}{2\hbar\sqrt{\pi}}}\left(\dfrac{2\mu\omega}{\hbar}x^2-1\right)e^{-\frac{\mu\omega}{2\hbar}x^2}$

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

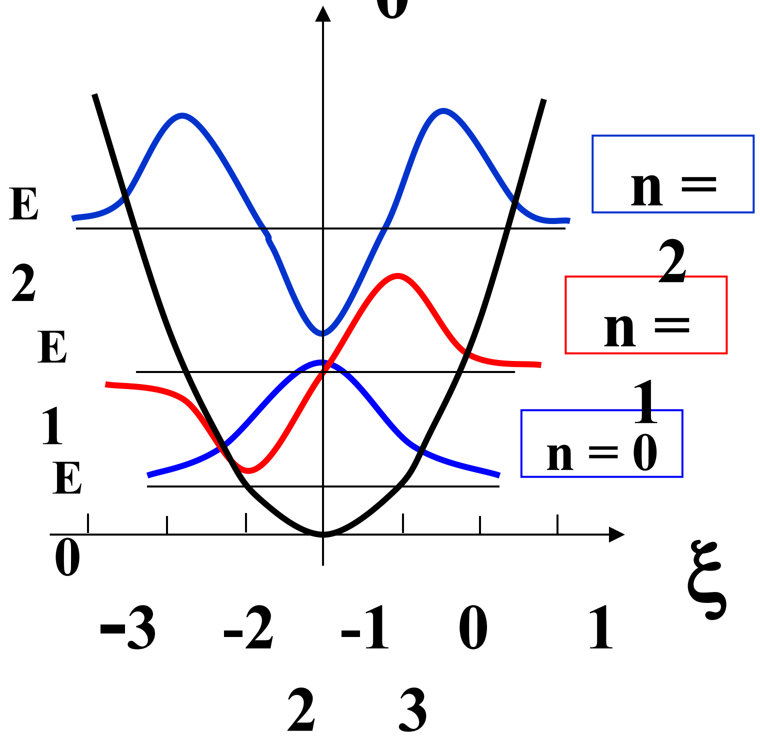
可以尝试猜测出最终结果，若ξ的最高次数为n，则对应的本征能量位(2*n+1)/2*hw

总结

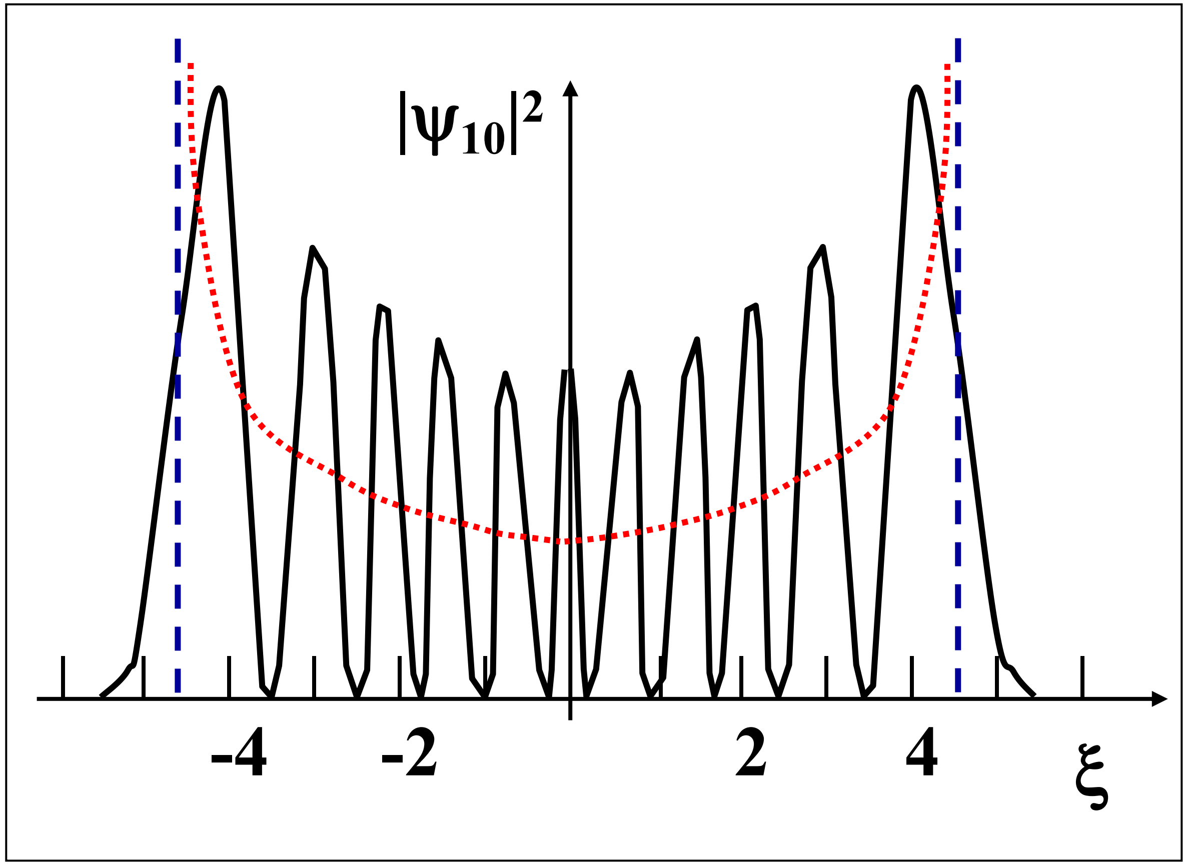
$$\to \left\{ \frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + [E - \frac{1}{2}\mu\omega^2 x^2] \right\}\psi(x) = 0$$



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



最终图像中的波峰数量正比于n，且两边峰更高，中间峰更矮。



从此图可以进行预测，当n足够大的时候最终的图像为一个抛物线的形状。

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

利用波函数的乘积的性质，分别求解！

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

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

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

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

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

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

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

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

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

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

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

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)

由于总离子数目固定，故两个维度的状态数确定后，即可自动确定最后一维的状态。

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

$$\text{坐标变换}\rightarrow\begin{cases}x'=x-x_0\\ \hat{p}=-i\hbar\frac{d}{dx}=-i\hbar\frac{d}{dx'}=\hat{p}'\end{cases}\qquad\rightarrow\hat{H}=\frac{\hat{p}^2}{2\mu}+\tfrac{1}{2}\mu\omega^2(x-x_0)^2-U_0$$

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

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

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

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

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

书上习题：

解：

$$\psi_0(x)=a_0e^{-\frac{1}{2}\alpha^2x^2}\qquad \alpha=\sqrt{\frac{m\omega}{\hbar}}\qquad \omega=\sqrt{\frac{k}{m}}$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}kx^2\right)\psi(x)=E\psi(x)$$

$$\psi_0'(x)=-\frac{1}{2}\alpha^2a_0 2xe^{-\frac{1}{2}\alpha^2x^2}$$

$$\psi_0''(x)=-\frac{1}{2}\alpha^2a_0 2e^{-\frac{1}{2}\alpha x^2}-\frac{1}{2}\alpha^2a_0 2x\left(-\frac{1}{2}\alpha^2 2xe^{-\frac{1}{2}\alpha x^2}\right)=-\alpha^2a_0e^{-\frac{1}{2}\alpha x^2}+\alpha^4a_0x^2e^{-\frac{1}{2}\alpha x^2}$$

$$\left(-\frac{\hbar^2}{2m}\left(-\alpha^2+\alpha^4x^2\right)+\frac{1}{2}kx^2\right)a_0e^{-\frac{1}{2}\alpha x^2}=Ea_0e^{-\frac{1}{2}\alpha x^2}$$

$$E=-\frac{\hbar^2}{2m}\left(-\alpha^2+\alpha^4x^2\right)+\frac{1}{2}kx^2\qquad E=\frac{\hbar^2}{2m}\left(\sqrt{\frac{m\omega}{\hbar}}\right)^2-\frac{\hbar^2}{2m}\left(\sqrt{\frac{m\omega}{\hbar}}\right)^4x^2+\frac{1}{2}kx^2$$

$$E=\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}-\frac{\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)^2x^2+\frac{1}{2}kx^2=\frac{1}{2}\hbar\omega-\frac{1}{2}m\omega^2x^2+\frac{1}{2}kx^2=\frac{1}{2}\hbar\omega$$