2023.12.5 一维谐振子

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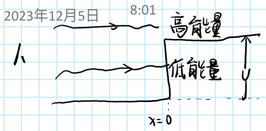

$E>U$.

$x<0$, $\psi_i = Ae^{ikx}$ 入射　$E=\frac{\hbar^2}{2m}k^2$, $E>U$

$\psi_r = Be^{-ikx}$ 反射　$k=\sqrt{\frac{2m}{\hbar^2}E}$.

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

$\psi_t = Ce^{ik'x}$　$k'=\sqrt{\frac{2m}{\hbar^2}(E-U)}$

波函数

在 $x=0$ 处，$\psi|_{x=0^-} = \psi|_{x=0^+}$ ①；$\psi'(x)|_{x=0^-} = \psi'(x)|_{x=0^+}$ ②

（原函数与导数在 $x=0$ 处连续）.

将上式综合讨论，$x<0$：$\psi(x)=Ae^{ikx}+Be^{-ikx}$

$x>0$：$\psi(x)=Ce^{ik'x}$

$\therefore \begin{cases} A+B=C & ① \\ A(ik)+B(-ik)=C(ik') & ② \end{cases} \Rightarrow \begin{cases} A=\frac{1}{2}(1+\frac{k'}{k})C \\ B=\frac{1}{2}(1-\frac{k'}{k})C. \end{cases}$ or $\begin{cases} C=\cdots A \\ B=\cdots A \end{cases}$

初始条件

$$j_i = -\frac{i\hbar}{2m}\left(\psi_i^*\frac{\partial}{\partial x}\psi_i - \psi_i\frac{\partial}{\partial x}\psi_i^*\right) = A^*A\frac{\hbar k}{m} \text{（入射流密度）}$$

$$j_t = -\frac{i\hbar}{2m}\left(\psi_t^*\frac{\partial}{\partial x}\psi_t - \psi_t\frac{\partial}{\partial x}\psi_t^*\right) = C^*C\frac{\hbar k'}{m} \text{（透射流密度）}$$

$$j_r = -\frac{i\hbar}{2m}\left(\psi_j^*\frac{\partial}{\partial x}\psi_j - \psi_j\frac{\partial}{\partial x}\psi_j^*\right) = B^*B\frac{\hbar k}{m} \text{（反射流密度）}$$

$\Rightarrow$ 透射系数 $T=j_t/j_i = \frac{C^*C}{A^*A}\frac{k'}{k} = \left|\frac{C^2}{A^2}\right|\frac{k'}{k} \overset{\text{初始条件}}{=\!=} \frac{4}{(1+\frac{k'}{k})^2}\frac{k'}{k} = \frac{4kk'}{(k+k')^2}$

反射系数 $R = j_r/j_i = \frac{B^*B}{A^*A} = \frac{(k-k')^2}{(k+k')^2}$

$$\boxed{T+R=1}$$

若 $E<U$，修正公式：

$x>0$ 时，$\psi_t = Ce^{-\beta x}$，$\beta=\sqrt{\frac{2m}{\hbar^2}(U-E)}$.

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

$\frac{d^2}{dx^2}\psi(x) = \beta^2\psi(x) \Rightarrow \psi(x) = Ce^{-\beta x}+De^{\beta x}$.

Let $D=0$. 得我们所需公式（衰减波）

$x<0$ 时 $\psi(x)=Ae^{ikx}+Be^{-ikx}$.

初始条件：$\begin{cases} A+B=C \\ ik(A-B)=-\beta C \end{cases} \Rightarrow \begin{cases} A=\frac{1}{2}(1+i\frac{\beta}{k})C \\ B=\frac{1}{2}(1-i\frac{\beta}{k})C. \end{cases}$ and $\begin{cases} C=\cdots A \\ B=\cdots A. \end{cases}$

计算 T 与 R：

反射与上例相同；$R=\frac{B^*B}{A^*A}=1$

透射系数：$T=j_t/j_i=0$.　$\boxed{R+T=1}$

when $j_t = -\frac{i\hbar}{2m}\left[C^*e^{-\beta x}\frac{\partial}{\partial x}(Ce^{-\beta x}) - Ce^{-\beta x}\frac{\partial}{\partial x}(C^*e^{-\beta x})\right]=0$

通量密度的计算：$\frac{\partial\rho}{\partial t}+\nabla\cdot\vec{j}=0$.

$\frac{\partial}{\partial t}[\Psi^*\Psi] = \frac{\partial\Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t}$.

利用薛定谔方程和复数共轭方程，我们有

$\frac{\partial}{\partial t}|\Psi|^2 = -\frac{\hbar}{2im}(\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*) = -\frac{\hbar}{2im}\nabla(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) = -\nabla\cdot\vec{j}$.

2、一维简谐振子

哈密顿量 $H=\begin{cases} \frac{1}{2}mv^2+\frac{1}{2}kx^2 & \text{宏观} \\ \frac{1}{2m}p^2+\frac{1}{2}kx^2 & \text{微观.} \end{cases}$

对应关系：
$E\to i\hbar\frac{\partial}{\partial t}$
$p\to\frac{\hbar}{i}\nabla$.

$\hat{H}=\frac{1}{2m}\hat{p}^2+\frac{1}{2}m\omega^2\hat{x} \Rightarrow \hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2$. (*)

以下为课件内容.

由(*)，化为 $H=\frac{1}{2}\hbar\omega\left[-\frac{\hbar}{m\omega}\frac{d^2}{dx^2}+\frac{m\omega}{\hbar}x^2\right]$

记 $\xi=\alpha x=\sqrt{\frac{m\omega}{\hbar}}x$，则 $H=\frac{1}{2}\hbar\omega\left[-\frac{d^2}{d\xi^2}+\xi^2\right]$.

由于 $H\psi=E\psi$，边界条件：$|\psi^2(x)|dx=0$，$x\to\infty$　即 $x\to\pm\infty$，$\psi(x)\to0$.

$\frac{1}{2}\hbar\omega\left[-\frac{d^2}{d\xi^2}\psi+\xi^2\psi\right]=E\psi$

(1) 若记 $\lambda=\frac{E}{\frac{1}{2}\hbar\omega}$，则 $-\frac{d^2}{d\xi^2}\psi+\xi^2\psi=\lambda\psi$ so that $\frac{d^2}{d\xi^2}\psi+(\lambda-\xi^2)\psi=0$.

先考虑边界条件　$x\to\pm\infty$，$\frac{d^2}{d\xi^2}\psi-\xi^2\psi=0 \Rightarrow \psi\propto\exp(\pm\frac{1}{2}\xi^2)$，又由于 $\exp(\frac{1}{2}\xi^2)\to+\infty$，故 $\psi\propto\exp(-\frac{1}{2}\xi^2)$！

故考虑 $\psi(\xi)=u(\xi)\exp(-\frac{1}{2}\xi^2)$ ⟶ 考虑了边界条件的形式.

$\frac{d\psi(\xi)}{d\xi}=\frac{du}{d\xi}\exp(-\frac{1}{2}\xi^2)-\xi u(\xi)\exp(-\frac{1}{2}\xi^2)$

$\frac{d^2\psi}{d\xi^2}=\frac{d^2u}{d\xi^2}\exp(-\frac{1}{2}\xi^2)-2\xi\frac{du}{d\xi}\exp(-\frac{1}{2}\xi^2)-u(\xi)\exp(-\frac{1}{2}\xi^2)+\xi^2u(\xi)\exp(-\frac{1}{2}\xi^2)$.

$\therefore \frac{d^2}{d\xi^2}\psi+(\lambda-\xi^2)\psi=\cdots\cdots=\left[\frac{d^2u}{d\xi^2}-2\xi\frac{du}{d\xi}+(\lambda-1)u\right]\exp(-\frac{1}{2}\xi^2)=0$.

$\therefore \frac{d^2}{d\xi^2}\psi+(\lambda-\xi^2)\psi=0$

$\frac{d^2u}{d\xi^2}-2\xi\frac{du}{d\xi}+(\lambda-1)u=0$. //$u''-2zu'+(\lambda-1)u=0$ 可解.

这里课件打错了，修正一下.

$u''-2zu'+(\lambda-1)u=0$

令 $u(z)=\sum_{k=0}^{+\infty}C_kz^k$　$u'(z)=\sum_{k=0}^{+\infty}kC_kz^{k-1}$，$u''(z)=\sum_{k=0}^{+\infty}(k+2)(k+1)C_{k+2}z^k$

$\therefore \sum_{k=0}^{+\infty}(k+2)(k+1)C_{k+2}z^k-\sum_{k=0}^{+\infty}2kC_kz^k+\sum_{k=0}^{+\infty}(\lambda-1)C_kz^k$

$=\sum_{k=0}^{+\infty}\{(k+2)(k+1)C_{k+2}-[2k-(\lambda-1)]C_k\}z^k=0$

$\Rightarrow$ 每一项系数为0，则 $C_{k+2}=\frac{2k-(\lambda-1)}{(k+2)(k+1)}C_k$

$\therefore u_1(z)=C_0+C_2z^2+\cdots$
$u_2(z)=C_1z+C_3z^3+\cdots$　} 初始条件 C_0，C_1.

解则演算查阅PPT.

由试写出.

$\therefore E=\frac{1}{2}\lambda\hbar\omega$，$E_n=\frac{1}{2}(2n+1)\hbar\omega \Rightarrow E_n=n\hbar\omega+\frac{1}{2}\hbar\omega$

$\psi_n(\xi)=C_nH_n(\xi)\exp(-\frac{1}{2}\xi^2)$.

$H_n(z)$（厄米特多项式的另一种写法）

$\exp(-s^2+2zs)=\sum_{n=0}^{+\infty}\frac{H_n(z)}{n!}s^n$

$H_n(z)=\frac{d^n}{ds^n}\exp(-s^2+2zs)\Big|_{s=0}=(-1)^n\exp(z^2)\frac{d^n}{dz^n}\exp(-z^2)$.

proof. 厄米特多项式正交.

$\exp(-t^2+2xt)\cdot\exp(-s^2+2zs)=\sum_{m,n=0}^{+\infty}\frac{H_m(z)}{m!}\frac{H_n(z)}{n!}t^ms^n$

又 $\exp(-s^2+2zs)\exp(-t^2+2zt)=\exp(2ts+z^2)\exp[-(t+s-z)^2]$

$=\sum_{m,n=0}^{+\infty}\frac{H_m(z)}{m!}\frac{H_n(z)}{n!}t^ms^n$

$\Rightarrow \exp(2ts)\exp[-(t+s-z)^2]=\cdots\exp(-z^2)$.

两侧同时对z积分.

积分过程见讲义.