量子序言

黑体辐射

能流密度 $J=\sigma T^4$. 斯特藩-玻尔兹曼定律

维恩位移定律 $\lambda_m T = 2898\,\mu m\cdot K$.

普朗克定律 $u(\nu,T)d\nu = \dfrac{8\pi\nu^2}{c^3}\dfrac{h\nu}{e^{\beta h\nu}-1}d\nu$.

$$u(\lambda,T)d\lambda = \frac{8\pi ch}{\lambda^5}\frac{1}{e^{\beta hc/\lambda}-1}d\lambda.$$

光电效应

电子吸收一个光子后逸出，频率低于 ν_c，不能激发(截止频率)

$$h\nu-\phi = T_{max}.$$

最大初动能通过遏止电势检测

$$T_{max}=eV_0$$

最大电流由光强决定(正比)

康普顿效应

能动量守恒：$E+m_0c^2 = E'+E_e$

$$\vec{p} = \vec{p}' + \vec{p}_e$$

相对论能动量关系：$E_e^2 = c^2p_e^2 + m_0^2c^4$ 电子

$E = cp$ 光子.

$$\Longrightarrow \lambda'-\lambda = \left(\frac{h}{m_0c}\right)(1-\cos\phi).$$

$\Lambda \equiv \dfrac{h}{m_0c}$ 康普顿波长.

氢原子.

里德伯公式：$\frac{1}{\lambda} = R_\infty\left(\frac{1}{m^2}-\frac{1}{n^2}\right)$ $n>m$.

里德伯常量

氢原子玻尔模型

$$E_n = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{2\eta a_0}\frac{1}{n^2} \qquad \left(\eta \equiv \frac{m_e}{\mu}?\right)$$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$$

物质波.

$$E=h\nu,\ p=\frac{h}{\lambda}=\hbar k.$$

$$\lambda = \frac{h}{p}$$

$$= \frac{hc}{\left[E_k(E_k+2m_0c^2)\right]^{1/2}} = \frac{h}{\sqrt{2m_0E_k}\left(1+\frac{E_k}{2m_0c^2}\right)^{1/2}}$$

极端相对论下 $\frac{1240\ \text{eV}\cdot\text{nm}}{E_k}$.

非相…电子 $\sqrt{\frac{1.504\ \text{eV}}{E_k}}\ \text{nm}$.

不确定关系.

$$\Delta x\Delta p \sim \hbar \geq \frac{1}{2}\hbar$$

薛定谔方程

$$E \rightarrow i\hbar\frac{\partial}{\partial t}, \quad \vec{p} \rightarrow -i\hbar\nabla,$$

$$E = \frac{p^2}{2m} + V$$

$$\Downarrow$$

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + U\psi$$

$$\Downarrow \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}).$$

薛定谔方程 $i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$ （非相对论）.

统计解释:

概率密度 $\rho = \psi^*(\vec{r},t)\psi(\vec{r},t)$.

概率流密度 $\vec{j} = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*)$

力学量由算子计算:

$\langle\hat{O}\rangle = \iiint \psi^*\hat{O}\psi\, d\vec{r}$ 均值

$\langle\hat{O}^2\rangle = \iiint \psi^*\hat{O}^2\psi\, d\vec{r}$

$\Delta\hat{O} = \langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2$ 涨落

$\hat{O}$代表任一力学量之算子.

归一化: $\int \psi^*\psi\, d\vec{r} = 1$.

定态薛定谔方程:

$\hat{H}\psi = E\psi$. E为$\hat{H}$的本征值.

（时间部分 $e^{-\frac{i}{\hbar}Et}$, 对概率等无影响）.

势阱

$$U=\begin{cases}0 & 0<x<a \\ \infty & \text{其它}.\end{cases}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \quad 即 \quad \frac{d^2\psi}{dx^2}+k^2\psi=0. \quad \left(k^2=\frac{2mE}{\hbar^2}\right).$$

边界 $\psi(0)=\psi(a)=0$；归一化

解：$\psi_n(x)=\sqrt{\frac{2}{a}}\sin(k_n x)$，$k_n=n\frac{\pi}{a}$. $E_n=\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$

势垒.(隧道效应)

$$U(x)=\begin{cases}U_0 & 0<x<a \\ 0 & \text{其它}.\end{cases}$$

$$\psi=\underset{(右行)}{Ae^{ik_1x}}+\underset{(左行)}{Be^{-ik_1x}} \qquad x<0. \qquad k_1^2=\frac{2mE}{\hbar^2}$$

$$\psi=Ce^{ik_2x}+De^{-ik_2x} \qquad 0<x<a. \qquad k_2^2=\frac{2m(E-U_0)}{\hbar^2}$$

$$\psi=Fe^{ik_3x} \qquad x>a. \qquad k_3^2=\frac{2m(E-U_1)}{\hbar^2}$$

(也有U_1)

$$R=\frac{|J_R|}{|J_I|}=\frac{B^*B\frac{\hbar k_1}{m}}{A^*A\frac{\hbar k_1}{m}}=\frac{|B|^2}{|A|^2}$$ + 边值条件.

$$T=\frac{|J_T|}{|J_I|}=\frac{F^*F\frac{\hbar k_3}{m}}{A^*A\frac{\hbar k_1}{m}}=\frac{|F|^2k_3}{|A|^2k_1}$$

隧道效应：$E<U_0$时 T仍非0. 粒子可能存在于势垒右侧.

阶梯势

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

$$\psi = Ae^{ikx} + Be^{-ikx} \qquad x<0. \quad k^2 = \frac{2mE}{\hbar^2}.$$

$$\psi = Ce^{ik'x} \ (E>U_0). \qquad \psi = De^{-\kappa x} \ (E<U_0) \quad x>0.$$

$$k'^2 = \frac{2m(E-U_0)}{\hbar^2} \qquad \kappa^2 = \frac{2mE(U_0-E)}{\hbar^2}$$

边界:

$$\begin{cases} \psi(0-) = \psi(0+) \\ \psi'(0-) = \psi'(0+). \end{cases}$$

$$C = \frac{2}{1+\frac{k'}{k}}A = \frac{2k}{k+k'}A.$$

$$B = \frac{1-\frac{k'}{k}}{1+\frac{k'}{k}} = \frac{k-k'}{k+k'}A.$$

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{k-k'}{k+k'}\right)^2.$$

$$T = \frac{|C|^2k'}{|A|^2k} = \frac{4kk'}{(k+k')^2}.$$

$$D = \frac{2}{1+\frac{i\kappa}{k}}A = \frac{2k}{k+i\kappa}A.$$

$$B = \frac{k-i\kappa}{k+i\kappa}A.$$

$$R = 1.$$

$$T = 0.$$ 右侧有波函数 但没有概率流.

简谐振子.

$$U = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2 \quad \left(\omega = \sqrt{\frac{k}{m}}\right)$$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2 = \frac{1}{2}\hbar\omega\left[-\frac{d^2}{d\xi^2} + \xi^2\right] \quad \left(\xi = \alpha x = \sqrt{\frac{m\omega}{\hbar}}x\right)$$

$$H\psi(x) = E\psi(x) \rightarrow \frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0. \quad \left(\lambda = \frac{E}{\frac{1}{2}\hbar\omega}\right)$$

$x \to \pm\infty$, $\psi \propto \exp(\pm\frac{1}{2}\xi^2) \to \psi \propto \exp(-\frac{1}{2}\xi^2)$.

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

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

Hermite方程.

级数解 $u(z) = \sum_{k=0}^{\infty} c_k z^k$. 代回方程.

$$c_{k+2} = \frac{2k-(\lambda-1)}{(k+2)(k+1)} c_k.$$

边界条件要求 $\lambda = 2n+1$ (收敛).

$$c_{k+2} = -\frac{2(n-k)}{(k+2)(k+1)} c_k.$$

$$c_{n+2} = c_{n+4} = \cdots = 0.$$

$u_1(z) = c_0 + c_2 z^2 + \cdots + c_n z^n$, n为偶

$u_2(z) = c_1 z + \cdots + c_n z^n$ 　　奇.

Hermite多项式

$$H_0(z) = 1$$

$$H_1(z) = 2z$$

$$H_2(z) = 4z^2 - 2$$

$$\vdots$$

解: $\psi_n(\xi) = C_n H_n(\xi)\exp(-\frac{1}{2}\xi^2)$, $\xi = \alpha x = \sqrt{\frac{m\omega}{\hbar}}x$

$E_n = n\hbar\omega + \frac{1}{2}\hbar\omega$. (三维: $E_N = (N + \frac{3}{2})\hbar\omega$

$C_n = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{\frac{1}{2}}$ 　　$N \equiv n_x + n_y + n_z$.)

(类)氢原子.

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze_s^2}{r}, \quad e_s^2 \equiv \frac{1}{4\pi\varepsilon_0}e^2$$

球坐标系中展开, 角度部分定义为 $-\frac{\hat{L}^2}{\hbar^2}$

径向部分和角度部分分离

角度部分: $\hat{L}^2 \underbrace{Y_{lm}(\theta,\varphi)}_{\text{球谐函数}} = \underbrace{\boxed{l(l+1)\hbar^2}}_{\hat{L}^2\text{的本征值}} Y_{lm}(\theta,\varphi)$

径向部分: 本征函数 $R_{nl}(r)$, 本征值(即能级)

$$E_n = -\frac{\mu Z^2 e_s^4}{2\hbar^2}\frac{1}{n^2}, \quad n = 1, 2, \cdots$$

n 为主量子数.

l 为角量子数. 取值 $l = 0, 1, \cdots, n-1$

m 为磁量子数, $m = -l, -(l-1), \cdots, l$.

简并度: 同一能级的状态数. $\sum_0^{n-1}\sum_{-l}^{l} 1 = n^2$.

跃迁只能发生于 $\Delta l = \pm 1$ 时.

$$E_n = -\frac{m_e Z^2 e_s^4}{\left(1+\frac{m_e}{m_p}\right)\cdot 2\hbar^2}\frac{1}{n^2} = -\frac{Z^2 e_s^2}{2\eta a_0}\frac{1}{n^2},$$

$$\eta = 1 + \frac{m_e}{m_p} = \frac{m_e}{\mu}$$

有效玻尔半径 $\eta a_0 = \frac{\hbar^2}{\mu e_s^2}$

概率密度: $w_{nl}(r)dr = r^2 dr \int d\Omega |\psi_{nlm}|^2$

$$= R_{nl}^2(r) r^2 dr$$

$$R_{nl} \sim e^{-\frac{1}{2}\rho} \rho^l L_{n-l-1}^{2l+1}(\rho); \quad \rho \equiv \frac{2Z}{na_0} r$$

$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$，本征值为 $m\hbar$，本征函数是球谐函数.

$\left(\hat{H} = \frac{\hat{L}_z^2}{2I} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\varphi^2} \right)$

X射线:

标识谱. 外层电子跃迁到内层产生的X射线.

外空穴向上跃迁.

能级 $E_n = \frac{(Z-1)^2 e_s^2}{2a_0}\frac{1}{n^2}$ (Z-1)由于内层电子屏蔽. (?)