2.3、若一晶体的相互作用能可以表示为

$$u(r) = -\frac{\alpha}{r^m} + \frac{\beta}{r^n}$$

试求：（1）平衡间距 r_0；

（2）结合能 W（单个原子的）；

（3）体弹性模量；

（4）若取 $m=2, n=10, r_0=3A, W=4eV$，计算 α 及 β 的值。

解：（1）求平衡间距 r_0

晶体内能 $U(r) = \frac{N}{2}(-\frac{\alpha}{r^m} + \frac{\beta}{r^n})$

平衡条件 $\left.\frac{dU}{dr}\right|_{r=r_0} = 0$，$-\frac{m\alpha}{r_0^{m+1}} + \frac{n\beta}{r_0^{n+1}} = 0$，$r_0 = (\frac{n\beta}{m\alpha})^{\frac{1}{n-m}}$

（2）单个原子的结合能

$W = -\frac{1}{2}u(r_0)$，$u(r_0) = \left.(-\frac{\alpha}{r^m} + \frac{\beta}{r^n})\right|_{r=r_0}$，$r_0 = (\frac{n\beta}{m\alpha})^{\frac{1}{n-m}}$

$$W = \frac{1}{2}\alpha(1-\frac{m}{n})(\frac{n\beta}{m\alpha})^{\frac{-m}{n-m}}$$

（3）体弹性模量 $K = (\frac{\partial^2 U}{\partial V^2})_{V_0} \cdot V_0$

晶体的体积 $V = NAr^3$，A 为常数，N 为原胞数目

晶体内能 $U(r) = \frac{N}{2}(-\frac{\alpha}{r^m} + \frac{\beta}{r^n})$

$$\frac{\partial U}{\partial V} = \frac{\partial U}{\partial r}\frac{\partial r}{\partial V} = \frac{N}{2}(\frac{m\alpha}{r^{m+1}} - \frac{n\beta}{r^{n+1}})\frac{1}{3NAr^2}$$

$$\frac{\partial^2 U}{\partial V^2} = \frac{N}{2}\frac{\partial r}{\partial V}\frac{\partial}{\partial r}[(\frac{m\alpha}{r^{m+1}} - \frac{n\beta}{r^{n+1}})\frac{1}{3NAr^2}]$$

$$\left.\frac{\partial^2 U}{\partial V^2}\right|_{V=V_0} = \frac{N}{2}\frac{1}{9V_0^2}[-\frac{m^2\alpha}{r_0^m} + \frac{n^2\beta}{r_0^n} - \frac{m\alpha}{r_0^m} + \frac{n\beta}{r_0^n}]$$

由平衡条件 $\left.\frac{\partial U}{\partial V}\right|_{V=V_0} = \frac{N}{2}(\frac{m\alpha}{r_0^{m+1}} - \frac{n\beta}{r_0^{n+1}})\frac{1}{3NAr_0^2} = 0$，得 $\frac{m\alpha}{r_0^m} = \frac{n\beta}{r_0^n}$

$$\left.\frac{\partial^2 U}{\partial V^2}\right|_{V=V_0} = \frac{N}{2}\frac{1}{9V_0^2}[-\frac{m^2\alpha}{r_0^m} + \frac{n^2\beta}{r_0^n}]$$

$$\left.\frac{\partial^2 U}{\partial V^2}\right|_{V=V_0} = \frac{N}{2}\frac{1}{9V_0^2}[-m\frac{m\alpha}{r_0^m} + n\frac{n\beta}{r_0^n}] = -\frac{N}{2}\frac{nm}{9V_0^2}[-\frac{\alpha}{r_0^m} + \frac{\beta}{r_0^n}]$$

$$U_0 = \frac{N}{2}(-\frac{\alpha}{r_0^m} + \frac{\beta}{r_0^n})$$

$$\left.\frac{\partial^2 U}{\partial V^2}\right|_{V=V_0} = \frac{mn}{9V_0^2}(-U_0)$$

体弹性模量 $K = |U_0|\frac{mn}{9V_0}$

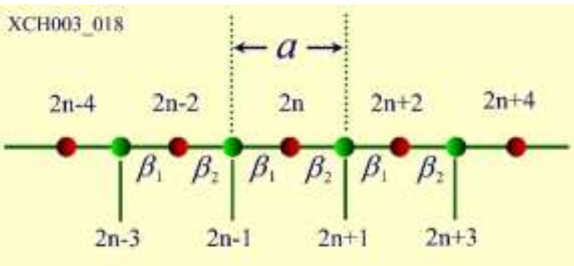
（4）若取 $m=2, n=10, r_0=3A, W=4\,eV$

$r_0 = (\frac{n\beta}{m\alpha})^{\frac{1}{n-m}}$， $W = \frac{1}{2}\alpha(1-\frac{m}{n})(\frac{n\beta}{m\alpha})^{\frac{-m}{n-m}}$

$\beta = \frac{W}{2}r_0^{10}$， $\alpha = r_0^2[\frac{\beta}{r_0^{10}} + 2W]$

$$\beta = 1.2\times10^{-95}\ eV\cdot m^{10}，\ \alpha = 9.0\times10^{-19}\ eV\cdot m^2$$

3.3、考虑一双子链的晶格振动，链上最近邻原子间的力常数交错地为 β 和 10β，两种原子质量相等，且最近邻原子间距为 $a/2$。试求在 $q=0, q=\pi/a$ 处的 $\omega(q)$，并粗略画出色散关系曲线。此问题模拟如 H_2 这样的双原子分子晶体。

答：（1）

浅色标记的原子位于 2n-1， 2n+1， 2n+3 ……；深色标记原子位于 2n， 2n+2， 2n+4 ……。
第 2n 个原子和第 2n＋1 个原子的运动方程：

$$m\ddot{\mu}_{2n} = -(\beta_1+\beta_2)\mu_{2n} + \beta_2\mu_{2n+1} + \beta_1\mu_{2n-1}$$
$$m\ddot{\mu}_{2n+1} = -(\beta_1+\beta_2)\mu_{2n+1} + \beta_1\mu_{2n+2} + \beta_2\mu_{2n}$$

体系 N 个原胞，有 2N 个独立的方程

方程的解：$\begin{matrix} \mu_{2n} = Ae^{i[\omega t-(2n)\frac{1}{2}aq]} \\ \mu_{2n+1} = Be^{i[\omega t-(2n+1)\frac{1}{2}aq]} \end{matrix}$，令 $\omega_1^2 = \beta_1 / m,\ \omega_2^2 = \beta_2 / m$，将解代入上述方程得：

$$(\omega_1^2+\omega_2^2-\omega^2)A-(\omega_1^2 e^{i\frac{1}{2}aq}+\omega_2^2 e^{-i\frac{1}{2}aq})B=0$$

$$(\omega_1^2 e^{-i\frac{1}{2}aq}+\omega_2^2 e^{i\frac{1}{2}aq})A-(\omega_1^2+\omega_2^2-\omega^2)B=0$$

A、B 有非零的解，系数行列式满足：

$$\begin{vmatrix} (\omega_1^2+\omega_2^2-\omega^2), & -(\omega_1^2 e^{i\frac{1}{2}aq}+\omega_2^2 e^{-i\frac{1}{2}aq}) \\ (\omega_1^2 e^{-i\frac{1}{2}aq}+\omega_2^2 e^{i\frac{1}{2}aq}), & -(\omega_1^2+\omega_2^2-\omega^2) \end{vmatrix}=0$$

$$(\omega_1^2+\omega_2^2-\omega^2)^2-(\omega_1^2 e^{i\frac{1}{2}aq}+\omega_2^2 e^{-i\frac{1}{2}aq})(\omega_1^2 e^{-i\frac{1}{2}aq}+\omega_2^2 e^{i\frac{1}{2}aq})=0$$

$$(\omega_1^2+\omega_2^2-\omega^2)^2-(\omega_1^2 e^{i\frac{1}{2}aq}+\omega_2^2 e^{-i\frac{1}{2}aq})(\omega_1^2 e^{-i\frac{1}{2}aq}+\omega_2^2 e^{i\frac{1}{2}aq})=0$$

因为 $\beta_1=\beta$、$\beta_2=10\beta$，令 $\omega_0^2=\omega_1^2=\frac{c}{m},\ \omega_2^2=\frac{10c}{m}=10\omega_0^2$ 得到

$$(11\omega_0^2-\omega^2)^2-(101+20\cos aq)\omega_0^4=0$$

两种色散关系：$\omega^2=\omega_0^2(11\pm\sqrt{20\cos qa+101})$

当 $q=0$ 时，$\omega^2=\omega_0^2(11\pm\sqrt{121})$，$\begin{matrix}\omega_+=\sqrt{22}\omega_0 \\ \omega_-=0\end{matrix}$

当 $q=\frac{\pi}{a}$ 时，$\omega^2=\omega_0^2(11\pm\sqrt{81})$，$\begin{matrix}\omega_+=\sqrt{20}\omega_0 \\ \omega_-=\sqrt{2}\omega_0\end{matrix}$

（2）色散关系图：