2. 一维复式格子,原子质量都为 $m$,原子统一编号,任一个原子与两最近邻的间距不同.力常数不同,分别为 $\beta_1$ 和 $\beta_2$,晶格常数为 $a$,求原子的运动方程及色散关系.

10. 设三维晶格一支光学波在 $q=0$ 附近,色散关系为 $\omega(q)=\omega_0-Aq^2$,证明该长光学波的模式密度

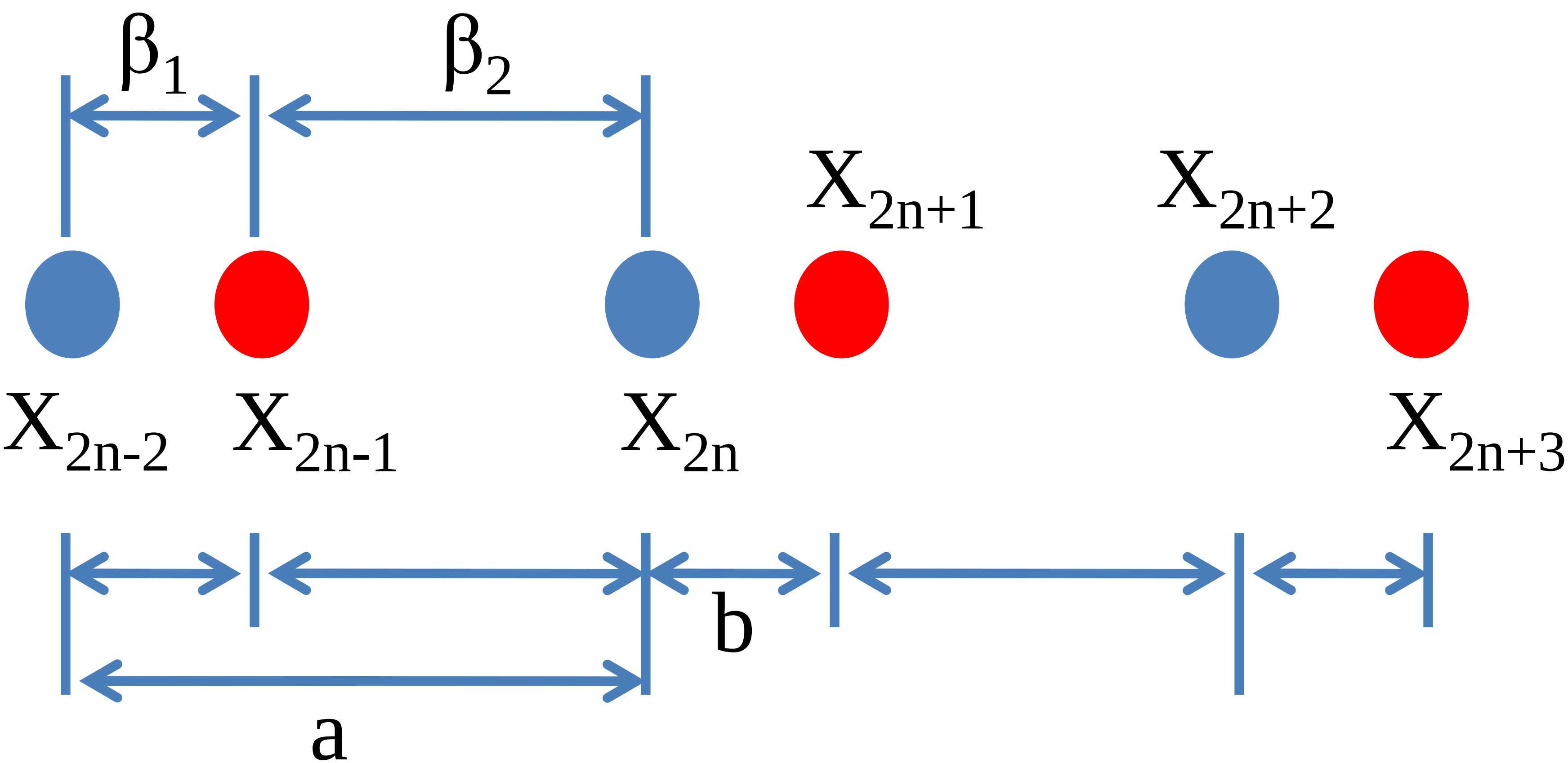
$$D(\omega)=\frac{V_c}{4\pi^2}\frac{1}{A^{3/2}}(\omega_0-\omega)^{1/2},\quad \omega<\omega_0.$$

15. 试用德拜模型,求 $T=0\mathrm{K}$ 时,晶格的零点振动能.

17. 按德拜近似,试证明高温时晶格热容

$$C_V=3Nk_B\left[1-\frac{1}{20}\left(\frac{\Theta_D}{T}\right)^2\right].$$

2. 一维复式格子，原子质量都为 $m$，原子统一编号，任一个原子与两最近邻的间距不同，力常数不同，分别为 $\beta_1$ 和 $\beta_2$，晶格常数为 $a$，求原子的运动方程及色散关系.



$$\begin{cases} F_{2n} = \beta_1(X_{2n+1} - X_{2n}) - \beta_2(X_{2n} - X_{2n-1}) \\ F_{2n+1} = \beta_2(X_{2n+2} - X_{2n+1}) - \beta_1(X_{2n+1} - X_{2n}) \end{cases}$$

$$\begin{cases} m\dfrac{d^2 X_{2n}}{dt^2} = \beta_1 X_{2n+1} + \beta_2 X_{2n-1} - (\beta_1 + \beta_2) X_{2n} \\ m\dfrac{d^2 X_{2n+1}}{dt^2} = \beta_2 X_{2n+2} + \beta_1 X_{2n} - (\beta_1 + \beta_2) X_{2n+1} \end{cases}$$

$$\left\{\begin{aligned}
X_{2n} &= Ae^{i\{\omega t - qna\}} \\
X_{2n+1} &= Be^{i\{\omega t - q[na+b]\}} \\
X_{2n+2} &= Ae^{i\{\omega t - q(n+1)a\}} \\
X_{2n-1} &= Be^{i\{\omega t - q[(n-1)a+b]\}}
\end{aligned}\right.$$

$$[(\beta_1 + \beta_2) - m\omega^2]A$$

$$-[\beta_1 e^{-iqb} + \beta_2 e^{-iq(b-a)}]B = 0$$

$$-[\beta_1 e^{iqb} + \beta_2 e^{-iq(a-b)}]A$$

$$+[-m\omega^2 + (\beta_1 + \beta_2)]B = 0$$

$$\begin{vmatrix} (\beta_1+\beta_2)-m\omega^2 & -[\beta_1 e^{-iqb}+\beta_2 e^{-iq(b-a)}] \\ -[\beta_1 e^{iqb}+\beta_2 e^{-iq(a-b)}] & -m\omega^2+(\beta_1+\beta_2) \end{vmatrix} = 0$$

$$m\omega^2 = (\beta_1+\beta_2) \pm$$

$$\sqrt{\beta_1^2+\beta_1\beta_2 e^{-iqa}+\beta_1\beta_2 e^{iqa}+\beta_2^2}$$

$$m\omega^2 = (\beta_1 + \beta_2) \pm$$

$$\sqrt{\beta_1^2 + 2\beta_1\beta_2\cos(qa) + \beta_2^2}$$

$$m\omega^2 = (\beta_1 + \beta_2) \pm$$

$$\sqrt{(\beta_1 + \beta_2)^2 - 4\beta_1\beta_2\sin^2\left(\frac{qa}{2}\right)}$$

$$m\omega^2 = (\beta_1 + \beta_2) \pm$$

$$\sqrt{(\beta_1 + \beta_2)^2 - 4\beta_1\beta_2 \sin^2\left(\frac{qa}{2}\right)}$$

$$\downarrow$$

$$\omega^2 = \frac{\beta_1 + \beta_2}{m}\left\{1 \pm \sqrt{1 - \frac{4\beta_1\beta_2}{(\beta_1 + \beta_2)^2}\sin^2\left(\frac{qa}{2}\right)}\right\}$$

10. 设三维晶格一支光学波在 $q=0$ 附近，色散关系为 $\omega(q)=\omega_0-Aq^2$，证明该长光学波的模式密度

$$D(\omega)=\frac{V_c}{4\pi^2}\frac{1}{A^{3/2}}(\omega_0-\omega)^{1/2},\quad \omega<\omega_0.$$

$$D_{(\omega)}=\frac{V_C}{(2\pi)^3}\frac{d\vec{q}}{d\omega}$$

$$d\vec{q}=4\pi q^2 dq$$

$$\Downarrow$$

$$D_{(\omega)}=\frac{V_C}{2\pi^2}q^2\frac{dq}{d\omega}$$

$$\omega = \omega_0 - Aq^2$$

$$\frac{d\omega}{dq} = -2Aq$$

$$q = \left( \frac{\omega_0 - \omega}{A} \right)^{1/2}$$

$$\frac{d\omega}{dq} = -2A^{1/2}\left[\omega_0 - \omega\right]^{1/2}$$

$$\frac{dq}{d\omega} = -\frac{1}{2} A^{-1/2} [\omega_0 - \omega]^{-1/2}$$

$$q^2 = \frac{\omega_0 - \omega}{A}$$

$$D_{(\omega)} = \frac{V_C}{2\pi^2} q^2 \frac{dq}{d\omega}$$

$$\left|\frac{dq}{d\omega}\right| = \frac{1}{2} A^{-1/2} [\omega_0 - \omega]^{-1/2}$$

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$$q^2 = \frac{\omega_0 - \omega}{A}$$

$$D_{(\omega)} = \frac{V_C}{2\pi^2} q^2 \frac{dq}{d\omega} = \frac{V_C}{4\pi^2} \frac{1}{A^{3/2}} (\omega_0 - \omega)^{1/2}$$

15. 试用德拜模型，求 $T=0K$ 时，晶格的零点振动能.

$$\overline{E}=\int_0^{\omega_m}\frac{1}{2}\hbar\omega\rho(\omega)d\omega$$

$$\omega=qv_p$$

$$D_{(\omega)} = \frac{V_C}{(2\pi)^3}\frac{d\vec{q}}{d\omega}$$

$$d\vec{q} = 4\pi q^2 dq$$

$$D_{(\omega)} = \frac{V_C}{2\pi^2} q^2 \frac{dq}{d\omega}$$

$$\omega = q v_p$$

$$\rho(\omega) = 3 \cdot \frac{V_C}{(2\pi)^3} \cdot 4\pi \frac{\omega^2}{v_p^3} = \frac{3V_C}{2\pi^2} \cdot \frac{\omega^2}{v_p^3}$$

$$\overline{E} = \int_0^{\omega_m} \frac{1}{2}\hbar\omega\rho(\omega)d\omega$$

$$\rho(\omega) = \frac{3V_C}{2\pi^2} \cdot \frac{\omega^2}{v_p^3}$$

$$\overline{E} = \frac{3\hbar V_C}{4\pi^2 v_p^3}\int_0^{\omega_m} \omega^3 d\omega = \frac{3V_C\hbar\omega_m^4}{16\pi^2 v_p^3}$$

$$\int_0^{\omega_m} \rho(\omega) d\omega = 3N \qquad \rho(\omega) = \frac{3V_C}{2\pi^2} \cdot \frac{\omega^2}{v_p^3}$$

$$\int_0^{\omega_m} \frac{3V_C}{2\pi^2 v_p^3} \omega^2 d\omega = 3N$$

$$\frac{3V_C}{6\pi^2 v_p^3} \omega_m^3 = 3N$$

$$\frac{3V_C}{6\pi^2 v_p^3}\omega_m^3 = 3N$$

$$\omega_m = \left(\frac{6N\pi^2 v_p^3}{V_C}\right)^{1/3}$$

$$\omega_m = \left( \frac{6N\pi^2 v_p^3}{V_C} \right)^{1/3}$$

$$\overline{E} = \frac{3V_C \hbar \omega_m^4}{16\pi^2 v_p^3} = \frac{9N\hbar}{8} \left( \frac{N\pi^2}{V_C} \right)^{1/3} v_p$$

17. 按德拜近似，试证明高温时晶格热容

$$C_V = 3Nk_B\left[1 - \frac{1}{20}\left(\frac{\Theta_D}{T}\right)^2\right].$$

$$C_V = \frac{3}{2\pi^2} \cdot \frac{V_C}{v_p^3} \int_0^{\omega_m} k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{\hbar\omega/k_B T}\omega^2}{\left[e^{\hbar\omega/k_B T} - 1\right]^2} d\omega$$

令 $x=\dfrac{\hbar\omega}{k_B T}$ ，则对应于 $\omega_m$ 的

$$x_m=\frac{\hbar\omega_m}{k_B T}=\frac{\theta_D}{T}$$

$\theta_D$ 被称为Debye温度

$$C_V=9Nk_B\left(\frac{T}{\theta_D}\right)^3\int_0^{\theta_D/T}\frac{e^x\cdot x^4}{\left(e^x-1\right)^2}dx$$

$$C_V = 9Nk_B\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{e^x \cdot x^4}{\left(e^x - 1\right)^2}\,dx$$

$$\frac{e^x}{\left(e^x - 1\right)^2} = \frac{1}{\left(e^{x/2} - e^{-x/2}\right)^2} \approx \frac{1}{\left(\frac{x}{2} + \frac{x}{2}\right)^2} = \left(\frac{1}{x}\right)^2$$

$$C_V = 9Nk_B\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} x^2 dx$$

$$= 3Nk_B\left(\frac{T}{\theta_D}\right)^3\left(\frac{\theta_D}{T}\right)^3 = 3Nk_B$$