固体物理作业 8 参考答案

1. 一维双原子链

记 k_1 左边的为 1 号, 右边的为 2 号，晶格常数 $a' = 2a$，势能

$$V = \frac{1}{2}\sum_x k_1[u_1(x) - u_2(x)]^2 + k_2[u_1(x) - u_2(x-a')]^2 \tag{1}$$

根据定义

$$V_{ij}(X) = \frac{\partial^2 V}{\partial u_1(x+X)\partial u_2(x)} \tag{2}$$

可根据(1)写出

$$\mathbf{V}(0) = \begin{bmatrix} k_1+k_2 & -k_1 \\ -k_1 & k_1+k_2 \end{bmatrix},\ \mathbf{V}(a') = \begin{bmatrix} 0 & -k_2 \\ 0 & 0 \end{bmatrix},\ \mathbf{V}(-a') = \begin{bmatrix} 0 & 0 \\ -k_2 & 0 \end{bmatrix}, \tag{3}$$

其余 $\mathbf{V}(X)$ 均为 0. 于是动力学矩阵

$$\mathbf{D}(q) = \frac{1}{M}\sum_X \mathbf{V}(X)e^{\mathbb{i}qX} \tag{4}$$

$$= \begin{bmatrix} k_1+k_2 & -k_1-k_2e^{\mathbb{i}qa'} \\ -k_1-k_2e^{-\mathbb{i}qa'} & k_1+k_2 \end{bmatrix} \tag{5}$$

对角化可得

$$\omega^2 = \frac{k_1+k_2}{M} \pm \frac{1}{M}\sqrt{(k_1+k_2\cos(qa'))^2 + k_2^2\sin^2(qa')} \tag{6}$$

$$= \omega_0^2 \pm \sqrt{\omega_0^2 - 4\nu^2\sin^2(qa'/2)} \tag{7}$$

其中 $\omega_0^2 = (k_1+k_2)/M$, $\nu^2 = \sqrt{k_1k_2}/M$.

2. 短程和长程相互作用：一维单原子链为例

(a)

由势能形式，容易写出

$$V(ma) = -K_{|m|}(m \neq 0), \quad V(0) = 2\sum_{m=1}^{\infty} K_m \tag{8}$$

于是可得

$$\omega^2 = D(q) = \frac{1}{M}\sum_{m=-\infty}^{\infty} V(ma)e^{\mathbb{i}qma} \tag{9}$$

$$= \frac{1}{M}\left[2\sum_{m=1}^{\infty} K_m + 2\sum_{m=1}^{\infty} K_m(e^{\mathbb{i}qma} + e^{-\mathbb{i}qma})\right] \tag{10}$$

$$= \frac{4}{M}\sum_{m=1}^{\infty} K_m \sin^2\left(\frac{mqa}{2}\right) \tag{11}$$

(b)

长波极限 $|qa| \ll 1$，有 $\sin^2(mqa/2) \approx \frac{1}{4}(qma)^2$，代入(11)可得

$$\omega = a\sqrt{\frac{1}{M}\sum_{m=1}^{\infty} m^2 K_m} \cdot |q| \tag{12}$$

(c)

取 $K_m = m^{-p}$，$1 < p < 3$，此时有

$$\omega^2 = \frac{4}{M}\sum_{m=1}^{\infty} m^{-p}\sin^2\left(\frac{mqa}{2}\right) \tag{13}$$

在长波极限 $|qa| \ll 1$ 下，可以化成黎曼积分

$$\omega^2 = \frac{4(qa)^{p-1}}{M}\sum_{m=1}^{\infty}(mqa)^{-p}\sin^2\left(\frac{mqa}{2}\right)\cdot(qa) \tag{14}$$

$$\sim \frac{4(qa)^{p-1}}{M}\int_0^{\infty} t^{-p}\sin^2(t/2)dt = -\frac{2(qa)^{p-1}}{M}\Gamma(1-p)\sin(\pi p/2) \tag{15}$$

故有 $\omega \propto |q|^{(p-1)/2}$.

(d)

(也不是很严谨...) 取 $p = 3$，$K_m = K/m^3$，代入(14)有

$$\omega^2 = 4\omega_0^2(qa)^2\sum_{m=1}^{\infty}(mqa)^{-3}\sin^2\left(\frac{mqa}{2}\right)\cdot(qa) \tag{16}$$

$$= 4\omega_0^2(qa)^2\left[(qa)^{-2}\sum_{m=1}^{M} m^{-3}\sin^2\left(\frac{mqa}{2}\right) + \int_{Mqa}^{\infty} t^{-3}\sin^2(t/2)dt\right] \tag{17}$$

其中 $M = \lfloor (qa)^{-1} \rfloor$. 第二项积分是一个常数，不属于领头项. 注意到 $\sin^2\left(\frac{mqa}{2}\right) = \sum_{n=1}^{\infty}\frac{(mqa)^{2n}}{(2n)!}$，则有

$$(qa)^{-2}\sum_{m=1}^{M} m^{-3}\sin^2\left(\frac{mqa}{2}\right) = \sum_{m=1}^{M}\frac{1}{4m} + \sum_{n=2}^{\infty}\sum_{m=1}^{M}\frac{(qa)^{2n-2}}{(2n)!}m^{2n-3} \tag{18}$$

对于 $n \geq 2$,

$$\sum_{m=1}^{M}\frac{(qa)^{2n-2}}{(2n)!}m^{2n-3} = \sum_{m=1}^{M}\frac{(qa)}{(2n)!}(qam)^{2n-2} \sim \int_0^1 \frac{dx}{(2n)!}x^{2n-2} = \frac{1}{(2n)!(2n-1)} \tag{19}$$

因此 (18) 式的第二项关于 n 的无穷级数收敛到一个常数，也不属于领头阶. 所以领头阶由级数

$$\sum_{m=1}^{M}\frac{1}{4m} \sim \frac{1}{4}(\log M + \gamma) \approx -\frac{1}{4}\log|qa| \tag{20}$$

给出. 最终 ω 的领头阶为

$$\omega = \omega_0\sqrt{-(qa)^2\log|qa|} \tag{21}$$

3. 简谐势系数和弹簧的劲度系数

(a)

由 $K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}') = K^{\alpha\beta}(\boldsymbol{R}'-\boldsymbol{R})$，可得

$$V = V_0 + \frac{1}{4}\sum_{\boldsymbol{R}\alpha,\boldsymbol{R}'\beta} K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}')[u^\alpha(\boldsymbol{R})u^\beta(\boldsymbol{R}) + u^\alpha(\boldsymbol{R}')u^\beta(\boldsymbol{R}') - u^\alpha(\boldsymbol{R})u^\beta(\boldsymbol{R}') - u^\alpha(\boldsymbol{R}')u^\beta(\boldsymbol{R})] \tag{22}$$

$$= V_0 + \frac{1}{2}\sum_{\boldsymbol{R}\alpha,\boldsymbol{R}'\beta} K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}')[u^\alpha(\boldsymbol{R})u^\beta(\boldsymbol{R}) - u^\alpha(\boldsymbol{R})u^\beta(\boldsymbol{R}')] \tag{23}$$

$$= V_0 + \frac{1}{2}\sum_{\boldsymbol{R}\alpha,\boldsymbol{R}'\beta} \left[\sum_{\boldsymbol{R}''} K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}'')\delta_{\boldsymbol{R}\boldsymbol{R}'} - K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}')\right] u^\alpha(\boldsymbol{R})u^\beta(\boldsymbol{R}') \tag{24}$$

故

$$V^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}') = \sum_{\boldsymbol{R}''} K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}'')\delta_{\boldsymbol{R}\boldsymbol{R}'} - K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}') \tag{25}$$

(b)

$$D^{\alpha\beta}(\boldsymbol{q}) = \frac{1}{M}\sum_{\boldsymbol{R}} V^{\alpha\beta}(\boldsymbol{R})e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}} \tag{26}$$

$$= \frac{1}{M}\sum_{\boldsymbol{R}} e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}}\left[\sum_{\boldsymbol{R}''} K^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}'')\delta_{\boldsymbol{R}0} - K^{\alpha\beta}(\boldsymbol{R})\right] \tag{27}$$

$$= \frac{1}{M}\sum_{\boldsymbol{R}} K^{\alpha\beta}(\boldsymbol{R})(1-e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}}) = \frac{1}{M}\sum_{\boldsymbol{R}} K^{\alpha\beta}(\boldsymbol{R})\left(1-\frac{e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}}+e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}}}{2}\right) \tag{28}$$

$$= \frac{1}{M}\sum_{\boldsymbol{R}} K^{\alpha\beta}(\boldsymbol{R})\left(1-\cos\boldsymbol{q}\cdot\boldsymbol{R}\right) \tag{29}$$

给定 $\boldsymbol{q}$，$D^{\alpha\beta}(\boldsymbol{q})$ 的本征值为 $\omega^2(\boldsymbol{q}s)$，由于对角化不改变矩阵的迹，有

$$\sum_s \omega^2(\boldsymbol{q}s) = \mathrm{Tr}\,\mathbf{D}(\boldsymbol{q}) = \frac{1}{M}\sum_{\boldsymbol{R}\alpha} K^{\alpha\alpha}(\boldsymbol{R})\left(1-\cos\boldsymbol{q}\cdot\boldsymbol{R}\right) \tag{30}$$

于是

$$\int \omega^2 g(\omega)\mathrm{d}\omega = \sum_s \int_{\mathrm{BZ}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d}\omega^2(\boldsymbol{q}s) \tag{31}$$

$$= \frac{1}{M}\sum_{\boldsymbol{R}\alpha} K^{\alpha\alpha}(\boldsymbol{R})\int_{\mathrm{BZ}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d}\left(1-\cos\boldsymbol{q}\cdot\boldsymbol{R}\right) \tag{32}$$

注意到

$$\int_{\mathrm{BZ}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d}\cos\boldsymbol{q}\cdot\boldsymbol{R} = \mathrm{Re}\int_{\mathrm{BZ}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d}e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}} = \frac{1}{V_c}\delta_{\boldsymbol{R}0}, \quad \int_{\mathrm{BZ}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d} = \frac{1}{V_c} \tag{33}$$

由于是单原子晶体，$n = 1/V_c$，代入 (32) 可得

$$\int \omega^2 g(\omega)\mathrm{d}\omega = \frac{1}{M}\sum_{\boldsymbol{R}\alpha} K^{\alpha\alpha}(\boldsymbol{R})\frac{1}{V_c}(1-\delta_{\boldsymbol{R}0}) \tag{34}$$

$$= \frac{n}{M}\sum_{\boldsymbol{R}\neq 0}\sum_{\alpha} K^{\alpha\alpha}(\boldsymbol{R}) \tag{35}$$