固体理论, Homework 05

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1 考虑一个包含四次非简谐项的一维振子链：

$$H=\sum_i \frac{P_i^2}{2M}+\sum_i\left[\frac{1}{2}M\omega_0^2(X_i-X_{i+1})^2+\alpha(X_i-X_{i+1})^4\right] \tag{1.1}$$

将上述经典哈密顿量用正则量子化写成声子的二次量子化形式。(提示：利用哈密顿量中的二次项进行正则量子化，用和课程中一样的方法引入声子产生/湮灭算符，再将四次项表示成产生湮灭算符的形式。)

Solution: Let

$$\begin{cases} P_i &= \dfrac{1}{\sqrt{N}}\sum_k \mathrm{e}^{\mathrm{i}\,kna}\,P_k \\ X_i &= \dfrac{1}{\sqrt{N}}\sum_k \mathrm{e}^{\mathrm{i}\,kna}\,X_k \end{cases} \tag{1.2}$$

thus, follow the textbook

$$\sum_i \frac{P_i^2}{2M}=\frac{1}{2M}\sum_k P_{-k}P_k \tag{1.3}$$

$$\sum_i \frac{1}{2}M\omega_0^2(X_i-X_{i+1})^2=\sum_k \frac{M\omega_k^2}{2}X_{-k}X_k \tag{1.4}$$

where

$$\omega_k^2=2\omega_0^2(1-\cos ka) \tag{1.5}$$

the rest term

$$\begin{aligned}(X_i-X_{i+1})^4 &= (X_i^2+X_{i+1}^2-X_iX_{i+1}-X_{i+1}X_i)^2 \\ &= X_{-k}X_kX_{-k}X_k\omega_k^4/\omega_0^4 \end{aligned} \tag{1.6}$$

Let

$$\tilde{P}_k=\frac{1}{\sqrt{2M\omega_k}}P_k \qquad \tilde{Q}_k=\sqrt{\frac{M\omega_k}{2}}X_k+\frac{\sqrt{\alpha\omega_k^3}}{\omega_0^2}X_kX_k \tag{1.7}$$

$$b_k=\tilde{Q}_k+\mathrm{i}\,\tilde{P}_k \qquad b_k^\dagger=\tilde{Q}_k-\mathrm{i}\,\tilde{P}_k \tag{1.8}$$

thus

$$H=\sum_k \omega_k(\tilde{P}_{-k}\tilde{P}_k+\tilde{Q}_{-k}\tilde{Q}_k) \tag{1.9}$$

$$=\sum_k \omega_k(b_k^\dagger b_k+\frac{1}{2}) \tag{1.10}$$

2　考虑课程中讨论的电子-晶格相互作用

$$H_{ei} = \sum_{ij} V_{ei}\left(\vec{r}_j - \vec{R}_i\right) \tag{2.1}$$

课上我们将 V_{ei} 展开到 $\vec{Q}_i$ 的线性项得到了电声子相互作用。将 V_{ei} 展开到下一阶（$\vec{Q}_i$ 的平方项），计算下一阶的电声子相互作用。

Solution:

$$\begin{aligned} H_{ei} &= \sum_{ij} V_{ei}(\vec{r}_j - \vec{R}_i^0) + \sum_{ij} \frac{\partial V_{ei}}{\partial R_i^0} \cdot \vec{Q}_i + \sum_{i,i'} \sum_j \vec{Q}_{i'} \frac{\partial^2 V_{ei}}{\partial R_i^0 \partial R_{i'}^0} \vec{Q}_i \\ &= \sum_{ij} V_{ei}(\vec{r}_j - \vec{R}_i^0) + \sum_{ij} \nabla_j V_{ei} \cdot \vec{Q}_i + \sum_{i,i'} \sum_j \vec{Q}_{i'} [\nabla_j \otimes \nabla_j] V_{ei} \vec{Q}_i \end{aligned} \tag{2.2}$$

Here by $[\nabla_j \otimes \nabla_j]V_{ei}$, we refer to a Hessian matrix of V_{ei} with respect to $\vec{r}_j$.
Do Fourier transformation

$$V_{ei} = \frac{1}{\sqrt{N}} \sum_k V_{ei}(\vec{k})\, \mathrm{e}^{\mathrm{i}\,\vec{k}\cdot(\vec{r}_j - \vec{R}_i^0)} \tag{2.3}$$

$$\nabla_j V_{ei} = \frac{1}{\sqrt{N}} \sum_k V_{ei}(\vec{k})\, \mathrm{e}^{\mathrm{i}\,\vec{k}\cdot(\vec{r}_j - \vec{R}_i^0)}\, \mathrm{i}\,\vec{k} \tag{2.4}$$

$$[\nabla_j \otimes \nabla_j] V_{ei} = \frac{1}{\sqrt{N}} \sum_k V_{ei}(\vec{k})\, \mathrm{e}^{\mathrm{i}\,\vec{k}\cdot(\vec{r}_j - \vec{R}_i^0)} [-\vec{k} \otimes \vec{k}] \tag{2.5}$$

thus

$$H_{e-ph}^1 = \sum_{q,L,\lambda} M_{qL\lambda}(b_q + b_{-q}^\dagger)\rho_{q+L} \tag{2.6}$$

$$\begin{aligned} H_{e-ph}^2 = &\sum_j \sum_{i,k,\lambda} \frac{1}{\sqrt{2MN\omega_{k\lambda}}} (b_{k\lambda}\lambda_k\, \mathrm{e}^{\mathrm{i}\,\vec{k}\cdot\vec{R}_i^0} + b_{k\lambda}^\dagger \lambda_k^*\, \mathrm{e}^{-\mathrm{i}\,\vec{k}\cdot\vec{R}_i^0}) \frac{1}{\sqrt{N}} \sum_{k''} V_{ei}(\vec{k}'')\, \mathrm{e}^{\mathrm{i}\,\vec{k}''\cdot(\vec{r}_j - \vec{R}_i^0)} [-\vec{k}'' \otimes \vec{k}''] \\ &\sum_{i',k',\lambda'} \frac{1}{\sqrt{2MN\omega_{k\lambda}}} (b_{k'\lambda'}\lambda_{k'}\, \mathrm{e}^{\mathrm{i}\,\vec{k}'\cdot\vec{R}_{i'}^0} + b_{k'\lambda'}^\dagger \lambda_{k'}^*\, \mathrm{e}^{-\mathrm{i}\,\vec{k}'\cdot\vec{R}_{i'}^0}) \end{aligned} \tag{2.7}$$