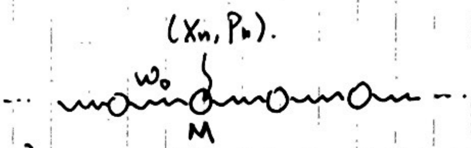
Lecture ~~8~~7 电子-晶格相互作用.

Ref. 教材 Chap. 11.

~~§11~~

1) 一维简谐振子链 §11.1.



$$H = \sum_n \frac{P_n^2}{2M} + \frac{1}{2} M \omega_0^2 \sum_n (X_n - X_{n+1})^2.$$

原子质量/位置/坐标, 大写字母. (电子, 小写字母).
一维位置用 n 表示 (避免和 i 重复).

经典 Hamiltonian ⟶ 正则量子化. (产生/湮灭算符).

* Fourier 变换得到正则模式:

$$\begin{cases} P_n = \frac{1}{\sqrt{N}} \sum_k e^{ikna} P_k & \longleftrightarrow \quad P_k = \frac{1}{\sqrt{N}} \sum_n e^{-ikna} P_n \\ X_n = \frac{1}{\sqrt{N}} \sum_k e^{ikna} X_k & \longleftrightarrow \quad X_k = \frac{1}{\sqrt{N}} \sum_n e^{-ikna} X_n. \end{cases}$$

Comments: - P_n, X_n 为实数 $\Leftrightarrow$ $P_k = P_k^*$; $X_{-k} = X_k^*$.

- 归一化, $\sum_n P_n^2 = \sum_k P_k^* P_k = \sum_k P_{-k} P_k$.

$\cancel{\sum_n (X_n - X_{n+1})^2 = \sum_n \sum_{k,k'}}$ $\sum_n X_n^2 = \sum_k X_{-k} X_k$.

$$\sum_n X_n X_{n+1} = \sum_n \sum_{k,k'} \frac{1}{N} e^{ikna} X_k e^{ik'(n+1)a} X_{k'}$$

$$= \sum_{k,k'} \underbrace{\frac{1}{N} \sum_n e^{i(k+k')na}}_{=\delta_{k+k',0}} e^{ik'a} X_k X_{k'}$$

$$= \sum_k e^{ika} X_{-k} X_k. = \sum_k e^{-ika} X_{-k} X_k.$$

$$\therefore \quad H = \sum_k \frac{P_{-k} P_k}{2M} + \frac{M\omega_0^2}{2} \sum_k X_k X_{-k} (2 - e^{ika} - e^{-ika})$$

$$= \frac{1}{2M} \sum_k P_{-k} P_k + \frac{M}{2} \sum_k \underbrace{2\omega_0^2 (1 - \cos ka)}_{= \omega_k^2} X_{-k} X_k$$

$$= \frac{1}{2M} \sum_k P_{-k} P_k + \sum_k \frac{M\omega_k^2}{2} X_{-k} X_k$$

w/ $\omega_k^2 = 2\omega_0^2 (1 - \cos ka)$.

$k \ll 1$: $\quad \omega_k^2 \approx 2\omega_0^2 (1 - \frac{1}{2} k^2 a^2) = \omega_0^2 k^2 a^2$

$\omega_k \approx \omega_0 a |k|$ 线性色散. (Goldstone 定理).

2) 正则量子化

量子力学对易关系：$[\hat{P}_n, \hat{X}_m] = -i\delta_{nm}$.

$$[\hat{P}_k, \hat{X}_{k'}] = \frac{1}{N}\sum_{nm}[\hat{P}_n, \hat{X}_m] e^{-ikna} e^{-ik'ma}$$
$$= \frac{1}{N}(-i)\sum_{nm}\delta_{nm} e^{-ikna} e^{-ik'ma}$$
$$= \frac{1}{N}(-i)\sum_{n} e^{-i(k+k')na}$$
$$= -i\delta_{k+k',0}.$$

或者 $[\hat{P}_k, \hat{X}_{-k'}] = -i\delta_{kk'}$.

在简正模式下，$H = \sum_k H_k$，$H_k = \frac{P_{-k}P_k}{2M} + \frac{M\omega_k^2}{2} X_{-k}X_k$.

相当于若干独立的谐振子模式

每个谐振子可用二次量子化写成产生/湮灭算符（之前的作业）.

令 $\tilde{Q}_k = \sqrt{\frac{M\omega_k}{2}} X_k$；$\tilde{P}_k = \frac{1}{\sqrt{2M\omega_k}} P_k$

$$[\tilde{P}_k, \tilde{Q}_{-k'}] = -\frac{i}{2}\delta_{kk'}.$$

令 $b_k = \tilde{Q}_k + i\tilde{P}_k$；$b_k^\dagger = \tilde{Q}_k - i\tilde{P}_k$.

$$[b_k, b_{k'}^\dagger] = [\tilde{Q}_k + i\tilde{P}_k, \tilde{Q}_{k'} - i\tilde{P}_{k'}]$$
$$= i[\tilde{P}_k, \tilde{Q}_{k'}] - i[\tilde{Q}_k, \tilde{P}_{k'}]$$
$$= i(-\tfrac{i}{2})\delta_{kk'} + i(-\tfrac{i}{2})\delta_{kk'} = \delta_{kk'}.$$

∴ $b_k^\dagger / b_k$ 为产生/湮灭算符. 产生/湮灭动量为 k 的声子.

$$H_k = \frac{1}{2M} 2M\omega_k \tilde{P}_{-k}\tilde{P}_k + \omega_k \tilde{Q}_{-k}\tilde{Q}_k$$
$$= \omega_k(\tilde{P}_{-k}\tilde{P}_k + \tilde{Q}_{-k}\tilde{Q}_k)$$

$\tilde{Q}_k = \frac{1}{2}(b_k + b_{-k}^\dagger)$. $\quad \tilde{Q}_{-k} = \frac{1}{2}(b_{-k} + b_k^\dagger) = \tilde{Q}_k^\dagger$.

$\tilde{P}_k = \frac{1}{2i}(b_k - b_{-k}^\dagger)$. $\quad \tilde{P}_{-k} = \frac{1}{2i}(b_{-k} - b_k^\dagger) = \tilde{P}_k^\dagger$.

$$\therefore H_k = \omega_k \frac{1}{4}(b_k^\dagger - b_{-k})(b_k - b_{-k}^\dagger) + \frac{\omega_k}{4}(b_{-k} + b_k^\dagger)(b_k + b_{-k}^\dagger)$$
$$= \frac{1}{4}\omega_k(b_k^\dagger b_k - b_k^\dagger b_{-k}^\dagger - b_{-k}b_k + b_{-k}b_{-k}^\dagger + b_{-k}b_k + b_{-k}b_{-k}^\dagger + b_k^\dagger b_k + b_k^\dagger b_{-k}^\dagger)$$
$$= \frac{1}{2}\omega_k(b_k^\dagger b_k + b_{-k}b_{-k}^\dagger) = \frac{1}{2}\omega_k(b_k^\dagger b_k + b_{-k}^\dagger b_{-k} + 1).$$

$$\therefore H = \sum_k H_k = \sum_k \omega_k(b_k^\dagger b_k + \underbrace{\tfrac{1}{2}}_{\text{零点能}})$$

$$X_n = \frac{1}{\sqrt{N}}\sum_k e^{ikna} X_k = \frac{1}{\sqrt{N}}\sum_k \sqrt{\frac{2}{M\omega_k}}\tilde{Q}_k$$
$$= \frac{1}{\sqrt{N}}\sum_k \frac{1}{\sqrt{2M\omega_k}}(b_k + b_{-k}^\dagger)e^{ikna}$$
$$= \frac{1}{\sqrt{N}}\sum_k \frac{1}{\sqrt{2M\omega_k}}(b_k e^{ikna} + b_k^\dagger e^{-ikna}).$$

含时演化: $X_n(t) = e^{iHt} X_n e^{-iHt}$

$$b_k(t) = e^{iHt} b_k e^{-iHt} = b_k e^{-i\omega_k t}$$

$\therefore \quad X_n(t) = \frac{1}{\sqrt{N}}\sum_k \frac{1}{\sqrt{2M\omega_k}} \left(b_k(t) e^{ikna} + b_k^+(t) e^{-ikna} \right)$

$$= \frac{1}{\sqrt{N}} \sum_k \frac{1}{\sqrt{2M\omega_k}} \left(b_k e^{ikna - i\omega_k t} + b_k^+ e^{-ikna + i\omega_k t} \right)$$

类似地: $P_n = \frac{1}{\sqrt{N}} \sum_k \sqrt{2M\omega_k}\, e^{ikna} \tilde{P}_k = \frac{-i}{\sqrt{N}} \sum_k \sqrt{\frac{M\omega_k}{2}} \left(b_k e^{ikna} - b_k^+ e^{-ikna} \right)$.

$\therefore \quad P_n(t) = \frac{-i}{\sqrt{N}} \sum_k \sqrt{\frac{M\omega_k}{2}} \left(b_k e^{ikna - i\omega_k t} + b_k^+ e^{-ikna + i\omega_k t} \right)$.

正则量子化: b_k, b_k^+ 为 X_n 的 Fourier "展开系数".

3) 声学声子: 3维模型的处理. 教材 §11.2.

从经典 Hamiltonian 出发, $H = \sum_i \frac{\vec{P}_i^2}{2M} + \sum_{i<j} V(\vec{R}_i - \vec{R}_j)$.

假设简单晶格: 1 atom / unit cell. 不考虑光学声子.

$V(\vec{R}_i - \vec{R}_j)$ 对平衡位置作展开: $\vec{R}_i = \vec{R}_i^0 + \vec{Q}_i$, s.t.

$$\left.\frac{\partial V}{\partial \vec{R}_i}\right|_{\vec{R}_i^0} = 0 \qquad V_0 = \text{常数}.$$

$$H = \sum_i \frac{\vec{P}_i^2}{2M} + \sum_{i<j} V(\vec{R}_i^0 - \vec{R}_j^0) + \frac{1}{2}\sum_{i<j} \frac{\partial^2 V}{\partial R^a \partial R^b} (Q_i^a - Q_j^a)(Q_i^b - Q_j^b)$$

简正模式: $H = \sum_{k\lambda} \frac{P_{-k\lambda} P_{k\lambda}}{2M} + V^0 + \frac{M}{2} \sum_{k,\lambda} \omega_{k\lambda}^2 \vec{Q}_{k\lambda} \cdot \vec{Q}_{k\lambda}$.

~~w/ $\vec{Q}_{k\lambda} = \frac{1}{\sqrt{N}}\sum_i$~~

w/ $\vec{Q}_i = \frac{1}{\sqrt{N}} \sum_{k\lambda} \hat{\lambda}_k e^{i\vec{k}\cdot\vec{R}_i^0} Q_{k\lambda} \leftrightarrow Q_{k\lambda} = \frac{1}{\sqrt{N}} \sum_i \hat{\lambda}_k \cdot \vec{Q}_i e^{-i\vec{k}\cdot\vec{R}_i^0}$.

正则量子化: $Q_{k\lambda} = \sqrt{\frac{2}{M\omega_{k\lambda}}} \tilde{Q}_{k\lambda} = \sqrt{\frac{2}{M\omega_{k\lambda}}} \frac{1}{2} (b_{k\lambda} + b_{-k\lambda}^+)$.

$$= \frac{1}{\sqrt{2M\omega_{k\lambda}}} (b_{k\lambda} + b_{-k\lambda}^+).$$

$\therefore \quad \vec{Q}_i(t) = \frac{1}{\sqrt{2MN\omega_{k\lambda}}} \sum_{k\lambda} \left[b_{k\lambda} \hat{\lambda}_k e^{i(\vec{k}\cdot\vec{R}_i^0 - \omega_{k\lambda} t)} + b_{k\lambda}^+ \hat{\lambda}_k^* e^{-i(\vec{k}\cdot\vec{R}_i^0 - \omega_{k\lambda} t)} \right]$

λ: 极化向量. $\sum_\lambda \hat{\lambda}_k^* \cdot \hat{\lambda}_k = 1$; $\hat{\lambda}_k^* = \hat{\lambda}_{-k}$.

1× 纵波, $\hat{\lambda}_k \parallel \vec{k}$

2× 横波: $\hat{\lambda}_k \perp \vec{k}$.

$$H = \sum_{k,\lambda} \omega_{k\lambda} \left(b_{k\lambda}^+ b_{k\lambda} + \frac{1}{2} \right).$$

4) 电-声子相互作用.

$$\vec{R}_i = \vec{R}_i^0 + \vec{Q}_i = \vec{R}_i^0 + \sum_{k\lambda}\frac{1}{\sqrt{2MN\omega_{k\lambda}}}\left(b_k\hat{\lambda}_k e^{i\vec{k}\cdot\vec{R}_i^0} + b_{k\lambda}^{+}\hat{\lambda}_k^{*}e^{-i\vec{k}\cdot\vec{R}_i^0}\right).$$

以此代入 $H_{ei} = \sum_{ij} V_{ei}(\vec{r}_j - \vec{R}_i)$；$\begin{cases}\vec{r}_j：\text{一次} \Rightarrow \text{二次量子化}.\\ \vec{R}_i：\text{经典场} \Rightarrow \text{正则量子化}.\end{cases}$

$$H_{ei} = \sum_{ij} V_{ei}(\vec{r}_j - \vec{R}_i^0) + \sum_{ij}\frac{\partial V_{ei}}{\partial \vec{R}_i^0}\cdot\vec{Q}_i$$

$$\left[\quad \frac{\partial V_{ei}}{\partial \vec{R}_i^0} = -\frac{\partial V_{ei}}{\partial \vec{r}_j} = -\nabla_j V_{ei}.\right]$$

$$H_{ei} = \sum_{ij} V_{ei}(\vec{r}_j - \vec{R}_i^0) - \sum_{ij}\vec{Q}_i\cdot\nabla_j V_{ei}(\vec{r}_j - \vec{R}_i^0).$$

* Fourier 变换至动量空间. $\vec{Q}_i = \sum_{k\lambda}\cdots(b_k^{+}\cdots + b_k^{+}\cdots)$

Vei 也作 Fourier 变换. 对一般量 $V_{ei}(\vec{r})$ （上式中 $\vec{r} = \vec{r}_j - \vec{R}_i^0$）.

$$V_{ei}(\vec{r}) = \sum_k V_{ei}(\vec{k})e^{i\vec{k}\cdot\vec{r}}$$

$$\therefore\ V_{ei}(\vec{r}_j - \vec{R}_i^0) = \frac{1}{\sqrt{N}}\sum_{k} V_{ei}(\vec{k})e^{i\vec{k}\cdot(\vec{r}_j - \vec{R}_i^0)}$$

而 $\nabla_j V_{ei}(\vec{r}_j - \vec{R}_i^0) = \frac{1}{\sqrt{N}}i\vec{k}\sum_{k} V_{ei}(\vec{k})e^{i\vec{k}\cdot(\vec{r}_j - \vec{R}_i^0)}$

$$\therefore\ H_{ei} = V^0 - \sum_{ij}\sum_{k\lambda}\frac{1}{\sqrt{2MN\omega_{k\lambda}}}\left(b_{k\lambda}\hat{\lambda}_k e^{i\vec{k}\cdot\vec{R}_i^0} + b_{k\lambda}^{+}\hat{\lambda}_k^{*}e^{-i\vec{k}\cdot\vec{R}_i^0}\right)\cdot\sum_{k'}\frac{i\vec{k}'}{\sqrt{N}}V_{ei}(\vec{k}')\, e^{i\vec{k}'\cdot(\vec{r}_j - \vec{R}_i^0)}$$

$$= V^0 - \sum_j\sum_{k\lambda k'}\frac{1}{\sqrt{2M\omega_{k\lambda}N}}\frac{1}{N}\sum_i V_{ei}(\vec{k}')(i\vec{k}')\cdot\left[b_{k\lambda}\hat{\lambda}_k e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_i^0} + b_{k\lambda}^{+}\hat{\lambda}_k^{*}e^{-i(\vec{k}+\vec{k}')\cdot\vec{R}_i^0}\right]e^{i\vec{k}'\cdot\vec{r}_j}$$

$$\frac{1}{N}\sum_i e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_i^0} = \sum_L \delta_{\vec{k}',\vec{k}+\vec{L}},\quad \vec{L}\text{ 为倒格矢}$$

这里 $\vec{k} \in$ 第一 B.Z. $\vec{k}' \in$ 全空间.

$$H_{ei} = V^0 - \sum_j\sum_{q\lambda L}\frac{1}{\sqrt{2MN\omega_{q,\lambda}}}V_{ei}(\vec{q}+\vec{L})\,(i(\vec{q}+\vec{L}))\cdot\hat{\lambda}_q(b_{q\lambda} + b_{-q\lambda}^{+})e^{i(\vec{q}+\vec{L})\cdot\vec{r}_j}$$

$$\sum_j e^{i\vec{k}\cdot\vec{r}_j} = \sum_j\int d\vec{r}\,\delta(\vec{r}-\vec{r}_j)e^{i\vec{k}\cdot\vec{r}}$$

一次 ⇒ 二次量子化：$\sum_j\delta(\vec{r}-\vec{r}_j) = \hat{n}(\vec{r})$.

$$\therefore\ \sum_j e^{i\vec{k}\cdot\vec{r}_j} = \int d\vec{r}\,\hat{n}(\vec{r})e^{i\vec{k}\cdot\vec{r}} = \hat{\rho}_k.$$

这里 $\hat{\rho}_q = \int d\vec{r}\,\hat{n}(\vec{r})e^{i\vec{q}\cdot\vec{r}} = \int d\vec{r}\,\psi^{+}(\vec{r})\psi(\vec{r})e^{i\vec{q}\cdot\vec{r}}$

$$= \int d\vec{r}\sum_{kk'}C_k^{+}e^{-i\vec{k}\cdot\vec{r}}C_{k'}e^{i\vec{k}'\cdot\vec{r}}e^{i\vec{q}\cdot\vec{r}}$$

$$= \sum_{kk'}C_k^{+}C_{k'}\int d\vec{r}\,e^{-i(\vec{k}-\vec{k}'-\vec{q})\cdot\vec{r}} = \sum_k C_{k+q}^{+}C_k.$$

$\therefore\ H_{ei} = V^0 - i\sum_{q\lambda L} \frac{1}{\sqrt{2M\omega_{q\lambda}N}} V_{ei}(\vec q+\vec L)\,(\vec q+\vec L)\cdot\hat\lambda_q\, \hat\rho_{q+L}\,(b_{q\lambda}+b^\dagger_{-q\lambda})$.

令 $M_{qL\lambda} = -i\frac{1}{\sqrt{2M\omega_{q\lambda}}}(\vec q+\vec L)\cdot\hat\lambda_q\cdot V_{ei}(\vec q+\vec L)$

$$\hat H_{e-ph} = \frac{1}{\sqrt N}\sum_{qL\lambda} M_{qL\lambda}(b_q+b^\dagger_{-q})\hat\rho_{q+L}$$

$$= \frac{1}{\sqrt N}\sum_{k,qL\lambda} M_{qL\lambda}\, C^\dagger_{k+q+L}C_k\,(b_q+b^\dagger_{-q})$$

5) 有效相互作用. §12.2.

$H = H_0 + H_{e-ph}$ 省略自旋

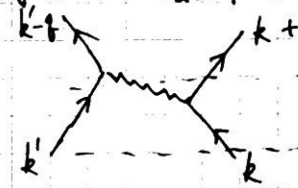
$$H_0=\sum_k \epsilon_k C_k^\dagger C_k + \sum_q \hbar\omega_q(b_q^\dagger b_q+\tfrac12)$$

$$H_{e-ph} = \frac{1}{\sqrt N}\sum_{kq} M_q\, C^\dagger_{k+q}C_k\,(b_q+b^\dagger_{-q})$$

为简化，略去自旋 σ，声子偏振 λ，电子/声子能带指标，$k,q\in 1^{st}$ B.Z.，$\vec L=0$

有效 e-e 相互作用：交换声子. 二阶微扰论

A)



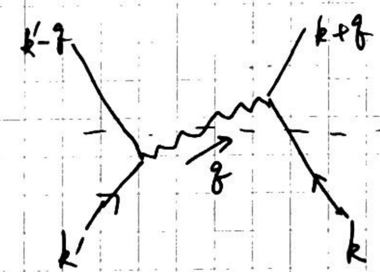
f: $C^\dagger_{k+q}C^\dagger_{k'-q}|0\rangle$ $\qquad E_f=\epsilon_{k'-q}+\epsilon_{k+q}$

中间: $C^\dagger_{k+q}C^\dagger_{k'}b^\dagger_{-q}|0\rangle$ $\qquad E=\epsilon_{k+q}+\epsilon_{k'}+\omega_q$

初 i: 2×电子@ k,k' $\quad C_k^\dagger C_{k'}^\dagger|0\rangle$ $\qquad E_i=\epsilon_k+\epsilon_{k'}$

$$H_A^{(2)} = \frac1N M_{-q}C^\dagger_{k'-q}C_{k'}b_{-q}\; M_q C^\dagger_{k+q}C_k b^\dagger_{-q}\cdot\frac12\left(\frac{1}{\epsilon_k-\epsilon_{k+q}-\omega_q}+\frac{1}{\epsilon_{k'-q}-\epsilon_{k'}-\omega_q}\right).$$

B)



f: $C^\dagger_{k'-q}C^\dagger_{k+q}|0\rangle$ $\qquad E_f=\epsilon_{k'-q}+\epsilon_{k+q}$

中间: $C^\dagger_{k'-q}C^\dagger_{k}b^\dagger_{q}|0\rangle$ $\qquad E=\epsilon_{k'-q}+\epsilon_k+\omega_q$

i: $C^\dagger_{k'}C^\dagger_{k}|0\rangle$ $\qquad E_i=\epsilon_k+\epsilon_{k'}$

$$H_B^{(2)}=\frac1N M_q C^\dagger_{k+q}C_k b_q\; M_{-q}C^\dagger_{k'-q}C_{k'}b^\dagger_q\;\frac12\left(\frac{1}{\epsilon_{k'}-\epsilon_{k'-q}-\omega_q}+\frac{1}{\epsilon_{k+q}-\epsilon_k-\omega_q}\right)$$

$H^{(2)}=H_A^{(2)}+H_B^{(2)}$ $\qquad (\langle b_q b_q^\dagger\rangle_0=\langle b_{-q}b^\dagger_{-q}\rangle_0=1$ @ $T=0)$.

$$=\frac12\frac1N\sum_{kk'q}|M_q|^2\, C^\dagger_{k+q}C_kC^\dagger_{k'-q}C_{k'}\,\frac12\Big(\frac{1}{\epsilon_k-\epsilon_{k+q}-\omega_q} + \frac{1}{\epsilon_{k+q}-\epsilon_k-\omega_q} + \frac{1}{\epsilon_{k'}-\epsilon_{k'-q}-\omega_q}+\frac{1}{\epsilon_{k'-q}-\epsilon_{k'}-\omega_q}\Big)$$

$\frac12$ 来自二次量子化 $H=\frac12\sum C^\dagger C^\dagger\langle|H^{(2)}|\rangle CC$

$\cancel{\frac12\sum_{kk'}\frac1N\sum_q|M_q|^2\left(\frac{\omega_q+\epsilon_k-\epsilon_{k+q}+\omega_q}{(\epsilon_k-\epsilon_{k+q})^2-\omega_q^2}\right)}$ $\qquad C^\dagger_{k+q}C_kC^\dagger_{k'-q}C_{k'}$

$$=\frac14\sum_{kk'}\frac1N\sum_q|M_q|^2\left[\frac{\epsilon_{k+q}-\epsilon_k-\omega_q+\epsilon_k-\epsilon_{k+q}-\omega_q}{(\epsilon_k-\epsilon_{k+q}-\omega_q)(\epsilon_{k+q}-\epsilon_k-\omega_q)}+\frac{-2\omega_q}{(\epsilon_{k'}-\epsilon_{k'-q}-\omega_q)(\epsilon_{k'-q}-\epsilon_{k'}-\omega_q)}\right]$$

$$=\frac1N\sum_{kk'q}|M_q|^2\frac{\omega_q}{\omega_q^2-(\epsilon_k-\epsilon_{k+q})^2}\,C^\dagger_{k+q}C^\dagger_{k'-q}C_{k'}C_k.$$

6) 声子格林函数.

自由玻色子:

定义 $G_{b\lambda}(\vec{q},\tau) = -T_\tau\langle b_{q\lambda}(\tau) b^\dagger_{q\lambda}(0)\rangle$

$$G_{b\lambda}(\vec{q},\omega_n) = \int_0^\beta d\tau\, G_{b\lambda}(\vec{q},\tau) e^{i\omega_n\tau} = \frac{1}{i\omega_n - \omega_{q\lambda}}.$$

考虑格林函数: $D(\vec{R}_i^0 - \vec{R}_j^0, \tau) = T_\tau\langle \vec{Q}_i(\tau)\cdot\vec{Q}_j(0)\rangle.$

$$= T_\tau\Big\langle \sum_{q\lambda}\frac{1}{\sqrt{2MN\omega_{q\lambda}}}\hat{\lambda}_q\,[b_{q\lambda}(\tau) + b^\dagger_{-q\lambda}(\tau)]e^{i\vec{q}\cdot\vec{R}_i^0}$$

$$\cdot\sum_{q'\lambda'}\frac{1}{\sqrt{2MN\omega_{q'\lambda'}}}\hat{\lambda}_{q'}[b_{q'\lambda'}(0) + b^\dagger_{-q'\lambda'}(0)]e^{i\vec{q}'\cdot\vec{R}_j}\Big\rangle$$

$$T_\tau\langle b_{q\lambda}(\tau)\, b^\dagger_{-q'\lambda'}(0)\rangle = -G_{b\lambda}(\vec{q},\tau)\,\delta_{q,-q'}\,\delta_{\lambda\lambda'}$$

$$T_\tau\langle b^\dagger_{-q\lambda}(\tau)\, b_{q'\lambda'}(0)\rangle = -G_{b\lambda}(\vec{-q},-\tau)\,\delta_{q,-q'}\,\delta_{\lambda\lambda'}$$

$$\therefore D(\vec{R}_i^0 - \vec{R}_j^0,\tau) = -\sum_{q\lambda}\frac{1}{2MN\omega_{q\lambda}}\hat{\lambda}_q^*\cdot\hat{\lambda}_q\,[G_{b\lambda}(\vec{q},\tau) + G_{b\lambda}(\vec{q},-\tau)]\,e^{i\vec{q}\cdot(\vec{R}_i^0 - \vec{R}_j^0)}$$

$$D(\vec{q},\omega_n) = -\sum_\lambda\frac{1}{2M\omega_{q\lambda}}[G_{b\lambda}(\vec{q},\omega_n) + G_{b\lambda}(\vec{q},-\omega_n)]$$

$$= -\sum_\lambda\frac{1}{2M\omega_{q\lambda}}\Big[\frac{1}{i\omega_n - \omega_{q\lambda}} + \frac{1}{-i\omega_n - \omega_{q\lambda}}\Big]$$

$$= \sum_\lambda\frac{1}{M(\omega_n^2 + \omega_{q\lambda}^2)}.$$

7) 路径积分量子化:

声子经典 Hamiltonian $H = \sum_{q\lambda}\frac{P^*_{q\lambda}P_{q\lambda}}{2M} + \frac{1}{2}M\sum_{q\lambda}\omega_{q\lambda}^2 Q^*_{q\lambda}Q_{q\lambda}.$

正则动量 $P_{q\lambda} = M\dot{Q}_{q\lambda} = M\frac{dQ_{q\lambda}}{dt}.$

$$L = \sum_{q\lambda}P^*_{q\lambda}\dot{Q}_{q\lambda} - H = \sum_{q\lambda}\frac{1}{2}M\Big|\frac{dQ_{q\lambda}}{dt}\Big|^2 - \frac{1}{2}M\sum_{q\lambda}\omega_{q\lambda}^2|Q_{q\lambda}|^2.$$

Feynman 路径积分: $Z = \int\mathcal{D}Q_{q\lambda}(t)\, e^{i\int dt\, L}$

Wick rotation: 实时 → 虚时 $\quad t\mapsto\tau = it.$

$$e^{i\int dt\,L} \mapsto e^{\int d\tau\sum_{q\lambda}[-\frac{1}{2}M|\frac{dQ_{q\lambda}}{d\tau}|^2 - \frac{1}{2}M\sum_{q\lambda}\omega_{q\lambda}^2|Q_{q\lambda}|^2]}$$

$$= e^{-\int d\tau\sum_{q\lambda}[\frac{1}{2}M|\frac{dQ_{q\lambda}}{d\tau}|^2 + \frac{1}{2}M\omega_{q\lambda}^2|Q_{q\lambda}|^2]}$$

$$S = \sum_{q\lambda}\frac{M}{2}\frac{dQ^*_{q\lambda}}{d\tau}\frac{dQ_{q\lambda}}{d\tau} + \frac{M}{2}\omega_{q\lambda}^2 Q^*_{q\lambda}Q_{q\lambda}$$

Fourier 变换: $Q_{q\lambda}(\tau)\to Q_{q\lambda}(\omega_n) = \int_0^\beta d\tau\, Q_{q\lambda}(\tau)e^{i\omega_n\tau}.$

周期性边界条件 $\Rightarrow \omega_n = \frac{2\pi n}{\beta}.$

$$\int\mathcal{D}Q_{q\lambda}(\tau) = \int\prod_n dQ^*_{q\lambda}(\omega_n)\,dQ_{q\lambda}(\omega_n)$$

高斯积分. $Z = \int\prod_n dQ^*_{q\lambda}(\omega_n)\,dQ_{q\lambda}(\omega_n)\, e^{-\sum_{\omega_n,q\lambda}\frac{1}{2}M(\omega_n^2 + \omega_{q\lambda}^2)|Q_{q\lambda}(\omega_n)|^2}$

$$\Rightarrow\langle Q^*_{q\lambda}(\omega_n)\,Q_{q\lambda}(\omega_n)\rangle = \frac{1}{M(\omega_n^2 + \omega_{q\lambda}^2)}.$$