FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023
21/11/2023
Aula 27

Aula passada

$$\boxed{H \;=\; \sum_{i,\alpha}\frac{P_{i\alpha}^2}{2M}+\frac{1}{2}\sum_{i\neq j} v\left(\mathbf{R}_i-\mathbf{R}_j\right)}$$

Expandindo em torno da posição de equilíbrio:

$$\mathbf{R}_i = \mathbf{R}_i^{(0)} + \mathbf{u}_i \qquad v\left(\mathbf{R}_i-\mathbf{R}_i\right) = v\left(\mathbf{R}_i^{(0)}-\mathbf{R}_i^{(0)}+\mathbf{u}_i-\mathbf{u}_j\right)$$

$$v\left(\mathbf{R}_i-\mathbf{R}_i\right) = v\left(\mathbf{R}_i^{(0)}-\mathbf{R}_i^{(0)}\right)+\frac{1}{2}\sum_{i,j,\alpha\beta}\left.\frac{\partial^2 v}{\partial R_{i\alpha}\partial R_{i\beta}}\right|_{\mathbf{R}_i^{(0)}-\mathbf{R}_i^{(0)}}\left(u_{i\alpha}-u_{j\alpha}\right)\left(u_{i\beta}-u_{j\beta}\right)$$

$$H \;=\; \sum_{i,\alpha}\frac{P_{i\alpha}^2}{2M}+\frac{1}{2}\sum_{i,j,\alpha,\beta} u_{i\alpha}C_{ij}^{\alpha\beta}u_{j\beta}$$

$$C_{ij}^{\alpha\beta} \;=\; C_{ij}^{\beta\alpha} = C_{ji}^{\alpha\beta}$$

$$\sum_j C_{ij}^{\alpha\beta} \;=\; 0$$

Aula passada

Transformando Fourier:

$$u_{i\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} u_{\mathbf{k},\alpha} \qquad u^{\dagger}_{\mathbf{k},\alpha} = u_{-\mathbf{k},\alpha}$$

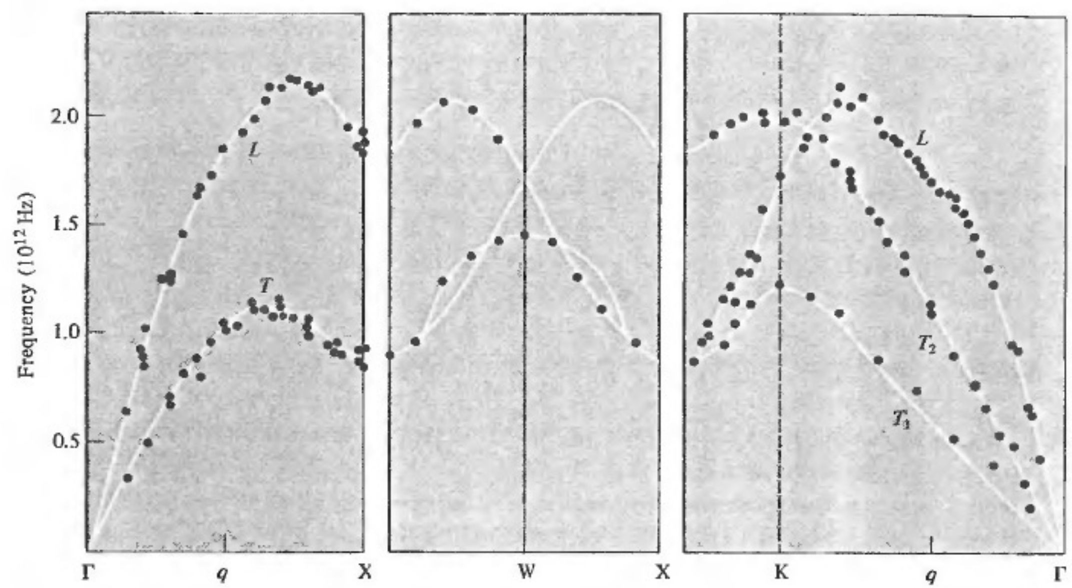
$$P_{i\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} P_{\mathbf{k},\alpha} \qquad P^{\dagger}_{\mathbf{k},\alpha} = P_{-\mathbf{k},\alpha}$$

$$H = \frac{1}{2M} \sum_{\mathbf{k},\alpha} P^{\dagger}_{\mathbf{k},\alpha} P_{\mathbf{k},\alpha} + \frac{1}{2} \sum_{\mathbf{k},\alpha,\beta} u^{\dagger}_{\mathbf{k},\alpha} C^{\alpha\beta}\left(\mathbf{k}\right) u_{\mathbf{k},\alpha}$$

Aula passada

Diagonalizando a matriz dinâmica:

$$\sum_{\beta} C^{\alpha\beta}(\mathbf{k})\, \epsilon_s^{\beta}(\mathbf{k}) = M\omega_s^2(\mathbf{k})\, \epsilon_s^{\alpha}(\mathbf{k})$$



$$\sum_{s} \epsilon_s^{\alpha}(\mathbf{k})\, \epsilon_s^{\beta}(\mathbf{k}) \;=\; \delta_{\alpha,\beta}$$

$$\sum_{\alpha} \epsilon_s^{\alpha}(\mathbf{k})\, \epsilon_{s'}^{\alpha}(\mathbf{k}) \;=\; \delta_{s,s'}$$

$$\epsilon_{s=1}^{\alpha}(\mathbf{k}) \;\parallel\; \mathbf{k} \;\; \text{(ramo acústico longitudinal)}$$

$$\epsilon_{s=2,3}^{\alpha}(\mathbf{k}) \;\perp\; \mathbf{k} \;\; \text{(ramos acústicos transversais)}$$

$$\vec{\epsilon}_s(\vec{k}) \propto |\vec{k}|$$

$$|\vec{k}| \to 0$$

Aula passada

Expandindo nos vetores de polarização:

$$u_{\mathbf{k},\alpha} = \sum_s u_{\mathbf{k},s}\epsilon_s^\alpha(\mathbf{k})$$

$$P_{\mathbf{k},\alpha} = \sum_s P_{\mathbf{k},s}\epsilon_s^\alpha(\mathbf{k})$$

$$H = \frac{1}{2M}\sum_{\mathbf{k},s} P^\dagger_{\mathbf{k},s}P_{\mathbf{k},s} + \frac{M}{2}\sum_{\mathbf{k},s}\omega_s^2(\mathbf{k})\,u^\dagger_{\mathbf{k},s}u_{\mathbf{k},s}$$

Definindo operadores de criação e destruição:

$$u_{\mathbf{k},s} = \frac{1}{\sqrt{2M\omega_s(\mathbf{k})}}\left(a_{\mathbf{k},s} + a^\dagger_{\mathbf{k},s}\right)$$

$$P_{\mathbf{k},s} = \frac{1}{i}\sqrt{\frac{M\omega_s(\mathbf{k})}{2}}\left(a_{\mathbf{k},s} - a^\dagger_{\mathbf{k},s}\right)$$

$$\left[a_{\mathbf{k},s}, a^\dagger_{\mathbf{k}',s'}\right] = \delta_{s,s'}\delta_{\mathbf{k},\mathbf{k}'}$$

$$\boxed{H = \sum_{\mathbf{k},s}\omega_s(\mathbf{k})\left(a^\dagger_{\mathbf{k},s}a_{\mathbf{k},s} + \frac{1}{2}\right)}$$

Interação elétron-fônon

HAMILTONIANO INTERAÇÃO ELÉTRON-REDE:

$$H_{e-R} = \sum_{ij} \tilde{V}(\vec{r}_i - \vec{R}_j)$$

$\vec{r}_i \rightarrow$ POSIÇÃO DO i-ÉSIMO ELÉTRON

$\vec{R}_j \rightarrow$ POSIÇÃO DO j-ÉSIMO ÍON

EXPANDINDO EM TORNO DE $R_j^{(0)}$:

$$\tilde{V}(\vec{r}_i - \vec{R}_j) = \tilde{V}(\vec{r}_i - \vec{R}_j^{(0)} - \vec{u}_j) \simeq \tilde{V}(\vec{r}_i - \vec{R}_j^{(0)}) - \vec{u}_j \cdot \vec{\nabla}\tilde{V}(\vec{r})\Big|_{\vec{r} = \vec{r}_i - \vec{R}_j^{(0)}}$$

A $O(u^2)$

$\sum_{ij} \tilde{V}(\vec{r}_i - \vec{R}_j^{(0)})$ = POTENCIAL DA REDE CRISTALINA QUE ATUA SOBRE OS ELÉTRONS.

$\Rightarrow$ A ESTRUTURA DE BANDAS E AS FUNÇÕES DE BLOCH DO ELÉTRONS

$$H_{e-R} = -\sum_{ij} \vec{u}_j \cdot \vec{\nabla} \tilde{V}(\vec{r}_i - \vec{R}_j^{(0)})$$

TRANSFORMADA DE FOURIER:

$$\tilde{V}(\vec{r}) = V \int \frac{d^3q}{(2\pi)^3} e^{-i\vec{q}\cdot\vec{r}} \, V(\vec{q})$$

TODO O ESPAÇO $\vec{q}$

$$\vec{\nabla}\tilde{V}(\vec{r}) = -iV \int \frac{d^3q}{(2\pi)^3} \vec{q} \, V(\vec{q}) \, e^{-i\vec{q}\cdot\vec{r}}$$

$$\Rightarrow H_{e-R} = iV \int \frac{d^3q}{(2\pi)^3} \sum_{ij} (\vec{q}\cdot\vec{u}_j) V(\vec{q}) \, e^{-i\vec{q}\cdot(\vec{r}_i - \vec{R}_j^{(0)})}$$

$$= iV \int \frac{d^3q}{(2\pi)^3} V(\vec{q}) \underbrace{\left[\sum_j (\vec{q}\cdot\vec{u}_j) e^{i\vec{q}\cdot\vec{R}_j^{(0)}}\right]}_{\sqrt{N}\,\vec{q}\cdot\vec{u}_{\vec{q}}} \left[\sum_i e^{-i\vec{q}\cdot\vec{r}_i}\right]$$

$$= i\sqrt{N} V \int \frac{d^3q}{(2\pi)^3} (\vec{q}\cdot\vec{u}_{\vec{q}}) V(\vec{q}) \left[\sum_i e^{-i\vec{q}\cdot\vec{r}_i}\right]$$

$$\sum_i e^{-i\vec{q}\cdot\vec{r}_i} = \int d^3r \underbrace{\sum_i \delta(\vec{r}-\vec{r}_i)}_{\rho(\vec{r}) = \text{OPERADOR DENSIDADE DOS ELÉTRONS}} e^{i\vec{q}\cdot\vec{r}} =$$

$$\rho(\vec{r}) = \sum_\alpha \psi^\dagger_\alpha(\vec{r})\,\psi_\alpha(\vec{r}) = \frac{1}{V}\sum_{\vec{k},\vec{p},\alpha} e^{-i(\vec{k}-\vec{p})\cdot\vec{r}}\, c^\dagger_{\vec{k},\alpha}\, c_{\vec{p},\alpha}$$

$$= \int d^3r\, e^{-i\vec{q}\cdot\vec{r}} \sum_\alpha \psi^\dagger_\alpha(\vec{r})\,\psi_\alpha(\vec{r}) = \sum_{\vec{k},\alpha} c^\dagger_{\vec{k}-\vec{q},\alpha}\, c_{\vec{k},\alpha} = \rho(-\vec{q})$$

USANDO: $\psi^\dagger_\alpha(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}}\, c^\dagger_{\vec{k},\alpha}$

USAREMOS QUE:

$$V \int_{\substack{\text{TODO}\\\text{ESPAÇO}\\\vec{q}}} \frac{d^3q}{(2\pi)^3} f(\vec{q}) = \sum_{\vec{K},\, \vec{q}\in BZ} f(\vec{K}+\vec{q})$$

E:

$$\vec{u}_{\vec{q}} = \sum_s \frac{1}{\sqrt{2M\omega_s(\vec{q})}} \left(a_{\vec{q},s} + a^\dagger_{-\vec{q},s}\right) \vec{\epsilon}_s(\vec{q}) = \vec{u}_{(\vec{K}+\vec{q})}$$

$$H_{e-ph} = i\sqrt{N} \sum_{\substack{\vec{k},\vec{K} \\ \vec{q}\in BZ \\ \alpha,s}} C^{\dagger}_{\vec{k}-\vec{K}-\vec{q},\alpha} C_{\vec{k},\alpha} V(\vec{K}+\vec{q}) \frac{(\vec{K}+\vec{q})\cdot\vec{\epsilon}_s(\vec{q})}{\sqrt{2M\omega_s(\vec{q})}} (a_{\vec{q},s}+a^{\dagger}_{-\vec{q},s})$$

PROCESSOS COM $\vec{K}\neq 0$ (UMKLAPP) GERALMENTE SÃO DESPREZÍVEIS EM BAIXAS ENERGIAS.

DESPREZANDO ESSES PROCESSOS:

$$\Rightarrow \boxed{H_{e-ph} = \sum_{\substack{\vec{k},\vec{q} \\ \alpha,s}} M^{s}_{\vec{q}} C^{\dagger}_{\vec{k}-\vec{q},\alpha} C_{\vec{k},\alpha} (a_{\vec{q},s}+a^{\dagger}_{-\vec{q},s})}$$

ONDE

$$M^{s}_{\vec{q}} = i\sqrt{N}\, \frac{V(\vec{q})\, \vec{q}\cdot\vec{\epsilon}_s(\vec{q})}{\sqrt{2M\omega_s(\vec{q})}}$$

SE $\vec{\epsilon}_s(\vec{q}) \perp \vec{q}$, $s=2,3$

$M^{s}_{\vec{q}} = 0$, $s=2,3$

E APENAS

$M^{1}_{\vec{q}} \neq 0$

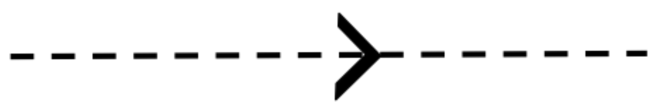
Resumo

$$H_{ph} = \sum_{\boldsymbol{q},s} \omega_s(\boldsymbol{q}) \left(a^{\dagger}_{\boldsymbol{q},s} a_{\boldsymbol{q},s} + \frac{1}{2} \right)$$

$$M_{\boldsymbol{q},s} = i\sqrt{N} \frac{\tilde{V}(\boldsymbol{q})\, \boldsymbol{q} \cdot \boldsymbol{\epsilon}_s(\boldsymbol{q})}{\sqrt{2M\omega_s(\boldsymbol{q})}}$$

$$H_{e-ph} = \sum_{\boldsymbol{kq}s\sigma} M_{\boldsymbol{q},s} c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma} \left(a_{\boldsymbol{q},s} + a^{\dagger}_{-\boldsymbol{q},s} \right)$$

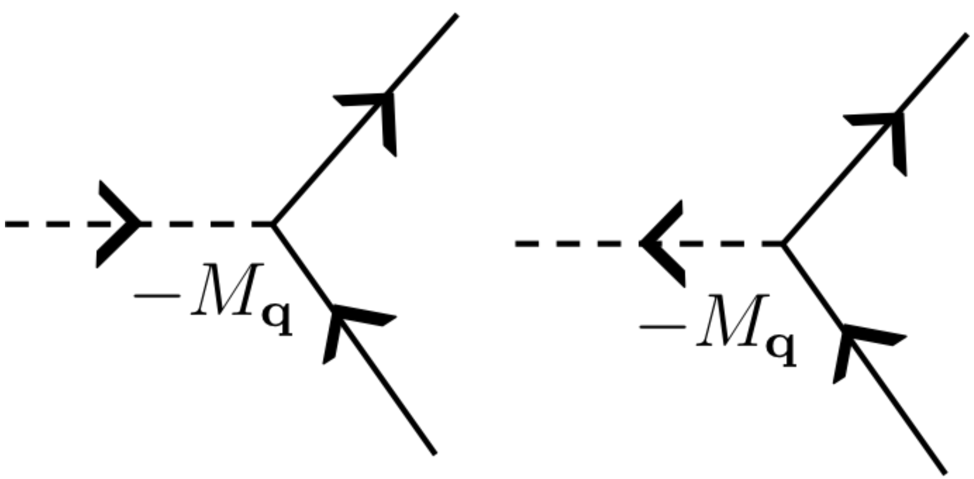
Função de Green dos fônons



$$\mathcal{D}^{(0)}(i\nu_n, \mathbf{q}) = \frac{1}{i\nu_n - \omega_s(\mathbf{q})}$$

$$\mathcal{G}^{(0)}(i\omega_n, \vec{k}) = \frac{1}{i\omega_n - \epsilon(\vec{k})}$$

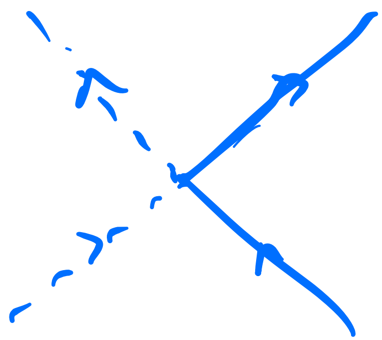
Vértice elétron-fônon



COMENTÁRIOS:

(i) SE $\tilde{V}(\vec{r}_i - \vec{R}_j^{(0)} - \vec{u}_j)$ FOR EXPANDIDO ATÉ A PRÓXIMA ORDEM:

$$\Longrightarrow c^{\dagger}_{\vec{k}+\vec{q},\alpha}\, c_{\vec{k},\alpha}\, (a_{\vec{q},s} + a^{\dagger}_{-\vec{q},s})(a_{\vec{q}',s'} + a^{\dagger}_{-\vec{q}',s'})\,\delta(\quad)$$

$\Longrightarrow$ 

(ii) ESTIMATIVAS DE GRANDEZAS DO PROBLEMA ELÉTRON-FÔNON:

- $\epsilon(\vec{k}) \sim \frac{k^2}{2m} \sim \frac{k_F^2}{2m} = E_F \simeq 1 - 10 \text{ eV} \cong 10^4 - 10^5 \text{ K}$

- $\omega_s(\vec{k}) \sim \sqrt{\frac{\text{"}k\text{"}}{M}} \sim \sqrt{\frac{\partial^2 \phi / \partial R^2}{M}}$ $\qquad \phi \sim E_F \qquad R \sim a =$ = PARÂMETRO DE REDE

$$\sim \sqrt{\frac{E_F}{M a^2}} = \sqrt{\frac{m}{M} \frac{E_F}{m a^2}} \qquad \frac{[(\hbar)^2]}{m a^2} \sim E_F$$

$$\omega_s(\vec{k}) \cong \sqrt{\frac{m}{M}} E_F \sim 10^{-2} E_F \sim \omega_D$$

$$\sim 10 \text{ meV}$$

$$\frac{m}{M} \sim 10^{-4}$$

$$\Rightarrow \frac{\omega_D}{E_F} \sim \sqrt{\frac{m}{M}} \sim 10^{-2} \ll 1$$

- $M \sim V\, u\, q$

$$V \sim E_F$$

$$u \sim \frac{1}{\sqrt{M\omega_s}} = \left(\frac{1}{M\sqrt{\frac{m}{M}E_F}}\right)^{1/2} = \frac{1}{(mM)^{1/4}E_F^{1/2}}$$

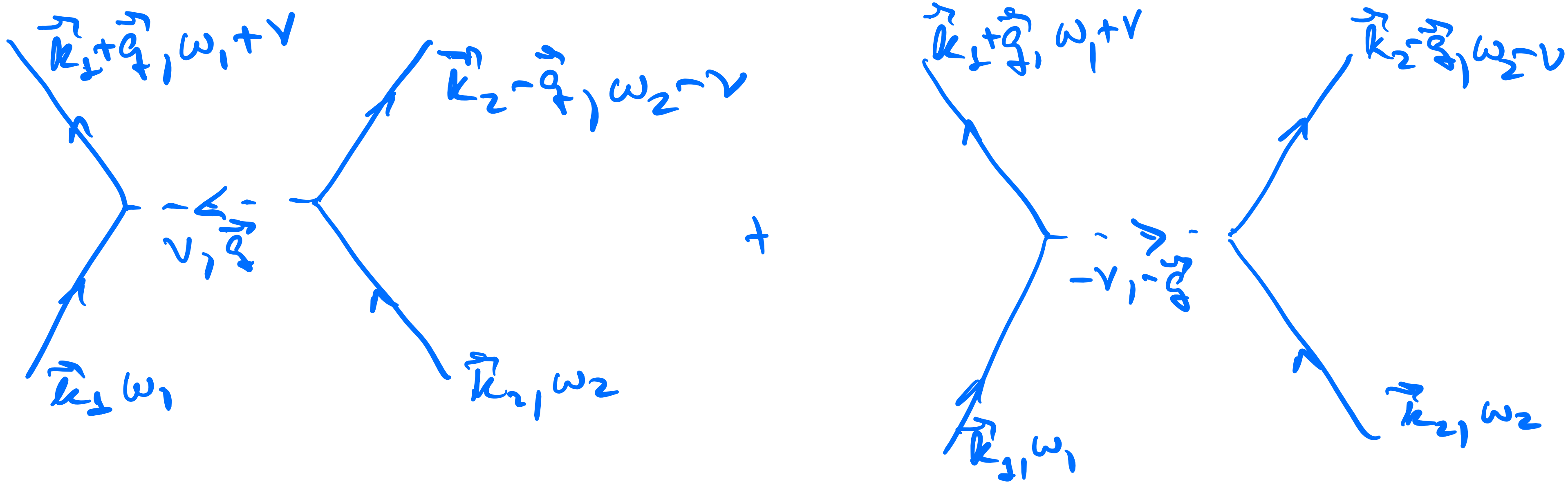
$$q \sim \frac{1}{a}$$

$$\Rightarrow M \sim E_F \frac{1}{a}\frac{1}{\sqrt{E_F}(mM)^{1/4}} = \frac{1}{(mM)^{1/4}}\sqrt{\frac{mE_F}{ma^2}}$$

$$= \frac{1}{(mM)^{1/4}}\sqrt{m}\,E_F = \left(\frac{m}{M}\right)^{1/4} E_F \sim 10^{-1} E_F$$

QUE NÃO É EXTREMAMENTE PEQUENO MAS JUSTIFICA UM TRATAMENTO PERTURBATIVO.

A INTERAÇÃO EFETIVA ENTRE OS ELÉTRONS DEVIDO À TROCA DE FÔNONS:



$$\Rightarrow (-M_{\vec{q}})^2 \left[-D^{(0)}(i\nu_n, \vec{q}) - D^{(0)}(-i\nu_n, -\vec{q}) \right]$$

$$= M_q^2 \left[\frac{-1}{i\nu_n - \omega_s(\vec{q})} - \frac{1}{-i\nu_n - \omega_s(\vec{q})} \right]$$

$$= -M_q^2 \left[\frac{-2\omega_s(q)}{-(i\nu_n)^2 + \omega_s^2(q)} \right] = -M_{\vec{q}}^2 \frac{2\omega_s(\vec{q})}{(i\nu_n)^2 - [\omega_s(\vec{q})]^2} = -V_{eff}(\vec{q}, \nu_n)$$

$$V_{eff}(\vec{q}, \nu_n) = M_q^2 \frac{2\omega_q}{(i\nu_n)^2 - \omega_q^2}$$ INTERAÇÃO RETARDADA

$$i\nu_n \longrightarrow \nu \implies V_{eff}(\vec{q}, \nu) = M_q^2 \frac{2\omega_q}{(\nu)^2 - \omega_q^2}$$

$$\nu \ll \omega_q \implies V_{eff}(\vec{q}, \nu) \simeq V_{eff}(\vec{q}, 0) = -\frac{M_q^2}{\omega_q} < 0$$

ATRATIVA !

$$\nu \gg \omega_q \implies V_{eff}(\vec{q}, \nu) > 0$$ REPULSIVA !

Hamiltoniano efetivo BCS