FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

1º Semestre de 2025

24/06/2025

Aula 27

Aula passada

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

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:

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

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

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

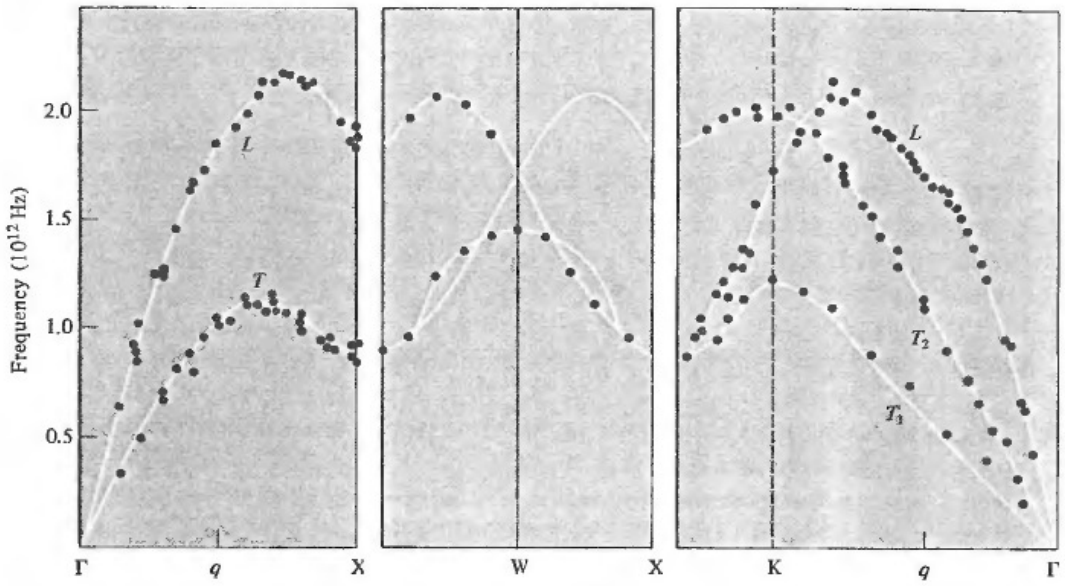
Aula passada

Diagonalizando a matriz dinâmica:

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

$$\sum_{s=1}^{3} \epsilon_s^{\alpha}(\mathbf{k})\,\epsilon_s^{\beta}(\mathbf{k}) = \delta_{\alpha,\beta}$$

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



Ao longo de direções de alta simetria:

$\vec{\epsilon}_{s=1}(\vec{k})\,\epsilon_{s=1}^{\alpha}(\mathbf{k}) \;\parallel\; \mathbf{k}$ (ramo acústico longitudinal)

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

$\omega_s(\vec{k}) \sim |\vec{k}|$

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

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

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

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

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

COMO ANTES:

$$\vec{R}_j = \vec{R}_j^{(0)} + \vec{u}_j$$

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

$\tilde{V}(\vec{r}_i - \vec{R}_j^{(0)})$: INTERAÇÃO DO i-ÉSIMO ELÉTRON COM A REDE EM EQUILÍBRIO

A SOLUÇÃO DO PROBLEMA DEFINIDO POR $\tilde{V}(\vec{r}_i - \vec{R}_j^{(0)})$ NOS DÁ A ESTRUTURA DE BANDAS E OS ESTADOS DE BLOCH.

VAMOS SUPOR QUE ESSE PROBLEMA JÁ FOI RESOLVIDO:

$$\Rightarrow \epsilon_m(\vec{k}), \quad \psi_{m\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_k^m(\vec{r})$$

O PRÓXIMO TERMO É:

$$H_{e\text{-}ph} = -\sum_{i,j} \vec{u}_j \cdot \vec{\nabla} \tilde{V}(\vec{r}_i - \vec{R}_j^{(0)})$$

TOMANDO A TRANSF. DE FOURIER DE $\tilde{V}(\vec{r})$:

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

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

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

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

$$n(\vec{r}) = \sum_\alpha \psi_\alpha^\dagger(\vec{r})\psi_\alpha(\vec{r})$$

$$\sum_i e^{i\vec{q}\cdot\vec{r}_i} = \int d^3r \overbrace{\sum_i \delta(\vec{r} - \vec{r}_i)}\, e^{i\vec{q}\cdot\vec{r}} = \int d^3r\, e^{i\vec{q}\cdot\vec{r}} n(\vec{r})$$

$$H_{e\text{-}ph} = -i\sqrt{n}\int \frac{d^3q}{(2\pi)^3} V(\vec{q})\, \vec{q}\cdot\vec{u}_{\vec{q}} \int d^3r\, e^{i\vec{q}\cdot\vec{r}}\, n(\vec{r})$$

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

ALÉM DISSO: $V\int \frac{d^3q}{(2\pi)^3} f(\vec{q}) = \sum_{\vec{q}\in BZ} f(\vec{q}+\vec{K})$ (2)

$\vec{K}$ REDE RECÍPROCA

$$\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\, n(\vec{r}) = \sum_\alpha \int d^3r\, e^{i\vec{q}\cdot\vec{r}}\, \psi^\dagger_\alpha(\vec{r})\,\psi_\alpha(\vec{r}) = (*)$$

IGNORANDO A BASE DE ESTADOS DE BLOCH E TRATANDO O GÁS DE ELÉTRONS COMO JELLIUM:

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

$$(*) \sum_\alpha \int d^3r\, e^{i\vec{q}\cdot\vec{r}} \sum_{\vec{q}'} \frac{e^{i\vec{q}'\cdot\vec{r}}}{\sqrt{V}}\, c^\dagger_{\vec{q}',\alpha} \sum_{\vec{p}} \frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}}\, c_{\vec{p},\alpha} = (*)$$

$$\frac{1}{V}\int d^3r\, e^{i(\vec{q}+\vec{q}'-\vec{p})\cdot\vec{r}} = \delta_{\vec{q}+\vec{q}',\vec{p}}$$

$$(*) = \sum_{\vec{p},\alpha} c^{+}_{\vec{p}-\vec{q},\alpha}\, c_{\vec{p},\alpha} \quad (3)$$

LEVANDO (1), (2) E (3) NO $H_{e\text{-}ph}$:

$$H_{e\text{-}ph} = -i\sqrt{N} \sum_{\vec{p},\vec{K},\vec{q},s,\alpha} V(\vec{K}+\vec{q})\, \frac{(\vec{q}+\vec{K})\cdot\vec{\epsilon}_s(\vec{q})}{\sqrt{2M\omega_s(\vec{q})}} \left(a_{\vec{q},s} + a^{+}_{-\vec{q},s}\right) \times$$

$$\times\, c^{+}_{\vec{p}-\vec{q}-\vec{K},\alpha}\, c_{\vec{p},\alpha}$$

TERMOS COM $\vec{K} \neq 0$ (PROCESSOS UMKLAPP) GERALMENTE SÃO DESPREZADOS (SÃO DE ALTA ENERGIA E GERALMENTE NÃO CONTRIBUEM MUITO). VAMOS FAZER $\vec{K}=0$.

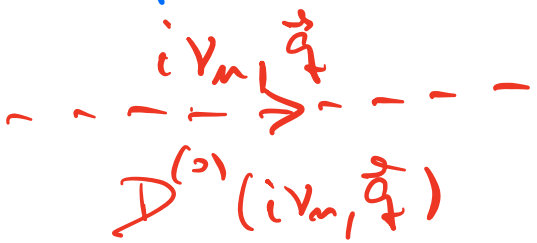
$$H_{e\text{-}ph} = \sum_{\substack{\vec{k},\vec{q} \\ s,\alpha}} M^{s}_{\vec{q}}\, c^{+}_{\vec{k}+\vec{q},\alpha}\, c_{\vec{k},\alpha} \left(a_{\vec{q},s} + a^{+}_{-\vec{q},s}\right)$$

↓ HAMILTONIANO DE INTERAÇÃO ELÉTRON-FÔNON

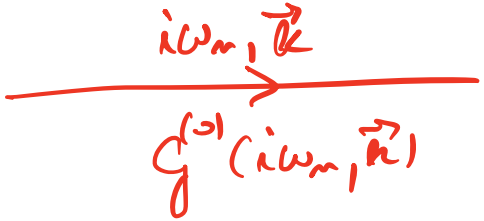
ONDE:

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

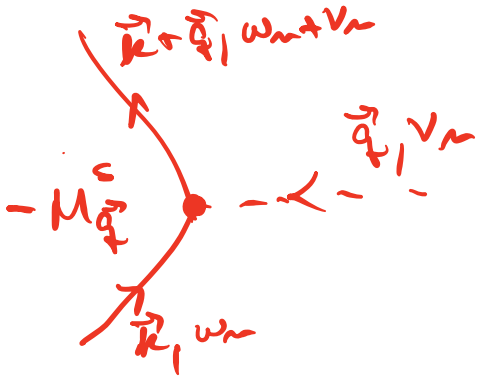
$$H_{ph} = \sum_{\vec{q},s} \omega^s_{\vec{q}}\, a^\dagger_{\vec{q},s}\, a_{\vec{q},s}$$

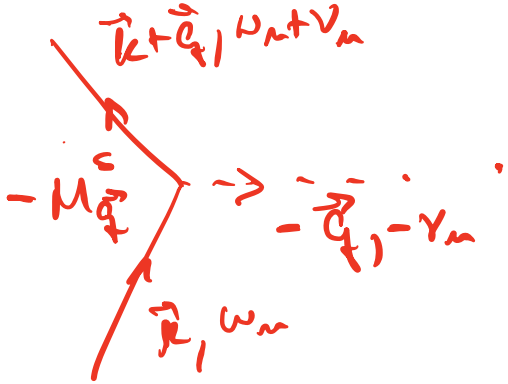


$$H_e = \sum_{\vec{k},\alpha} \epsilon(\vec{k})\, c^\dagger_{\vec{k},\alpha}\, c_{\vec{k},\alpha}$$



VERTICES:





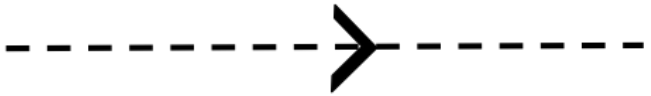
Resumo

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

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

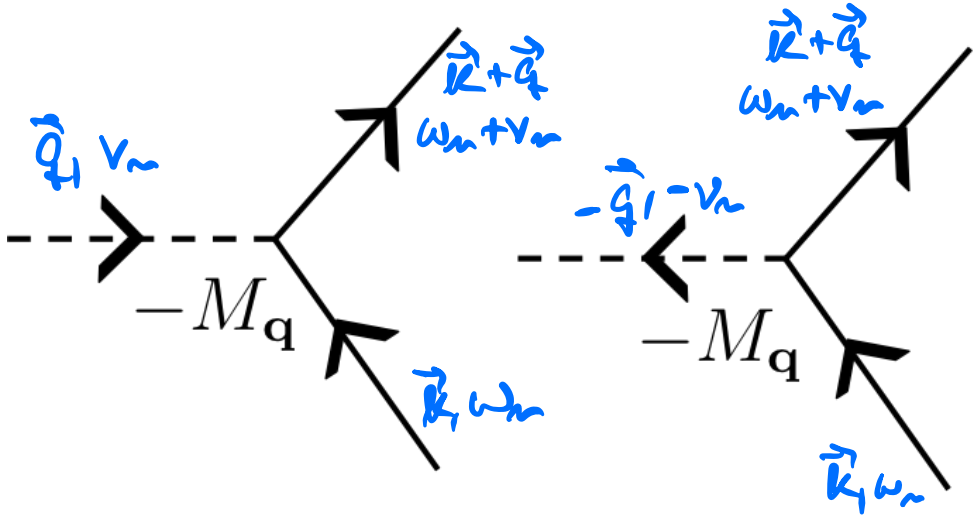
$$H_{e-ph} = \sum_{\boldsymbol{k}\boldsymbol{q}s\sigma} M_{\boldsymbol{q},s} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma} \left(a_{\boldsymbol{q},s} + a^\dagger_{-\boldsymbol{q},s} \right)$$

Função de Green dos fônons



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

Vértice elétron-fônon

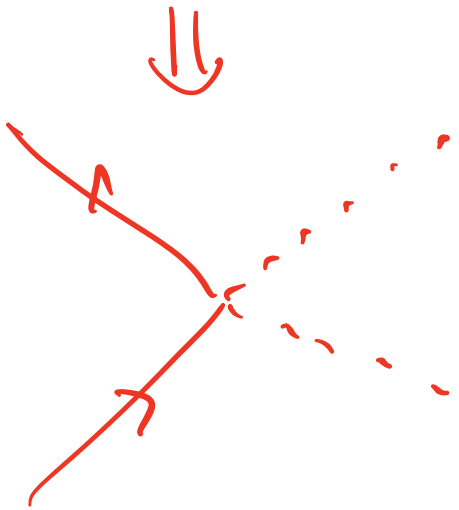


- LEVANDO EM CONTA OUTRAS BANDAS

$$c_{\vec{k},\alpha} \longrightarrow c^{n}_{\vec{k},\alpha}$$

- EM ORDENS SUPERIORES, P. EX., $u^{\alpha} u^{\beta}$:

$$c^{\dagger} c (a + a^{\dagger})(a + a^{\dagger})$$



ESTIMATIVAS DE VALORES:

- $\omega_s(q) \sim \sqrt{\frac{"k"}{M}}$ $\qquad "k" \sim \frac{\partial^2 \vartheta}{\partial \lambda^2} \sim \frac{\vartheta}{a_0^2} \sim \frac{E_F}{a_0^2}$

ONDE $E_F \sim 1-10\ eV$

$a_0 \sim 1\ \text{Å}$

$$\omega_s \sim \sqrt{\frac{E_F}{M a_0^2}} = \sqrt{\frac{m E_F}{M \underbrace{m a_0^2}_{\sim E_F^2}}}$$

$$\frac{1}{m a_0^2} = \frac{\hbar^2}{m a_0^2} \sim E_F$$

$$= E_F \sqrt{\frac{m}{M}} \simeq 10^{-2} E_F = \omega_D \Rightarrow \boxed{\frac{\omega_D}{E_F} \sim 10^{-2}}$$

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

- $M_q^s \sim V\, q\, u$

$$u \sim \frac{1}{\sqrt{M\omega_s}}$$

$$q \sim \frac{1}{a_0}$$

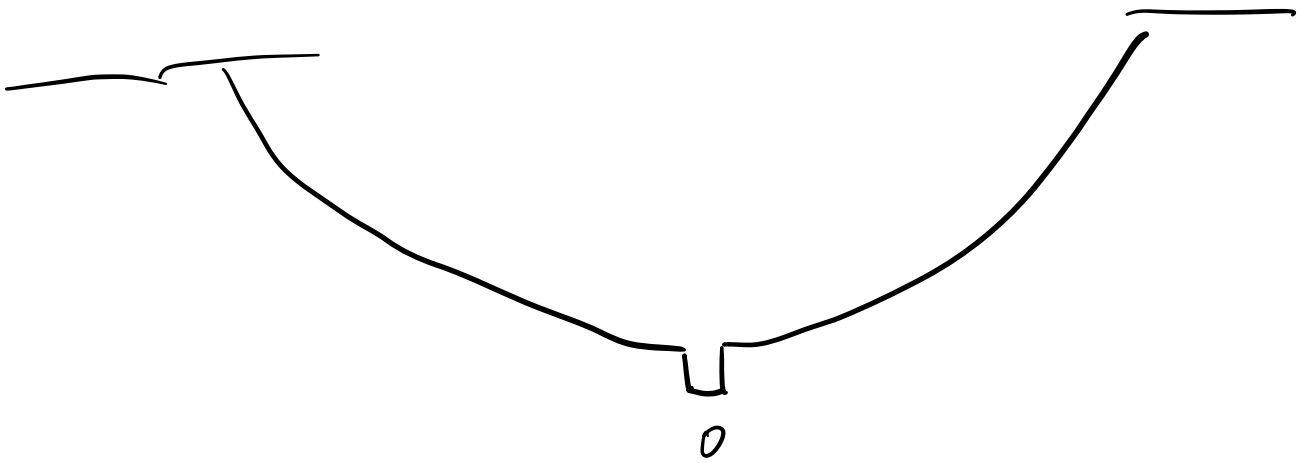
$$V \sim E_F$$

$$(uq)^2 \sim \frac{1}{M\omega_D a_0^2} = \frac{m}{M}\,\frac{1}{\omega_D}\,\frac{1}{m a_0^2}$$

$$= \frac{E_F}{\omega_D}\,\frac{m}{M} = \sqrt{\frac{m}{M}}\,\frac{m}{M}$$

$$= \sqrt{\frac{m}{M}} \Rightarrow uq \sim \left(\frac{m}{M}\right)^{1/4}$$

$$\Rightarrow M_q^s \sim \left(\frac{m}{M}\right)^{1/4} E_F \sim 10^{-1} E_F \Rightarrow \boxed{\frac{M_q^s}{E_F} \sim 10^{-1}}$$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