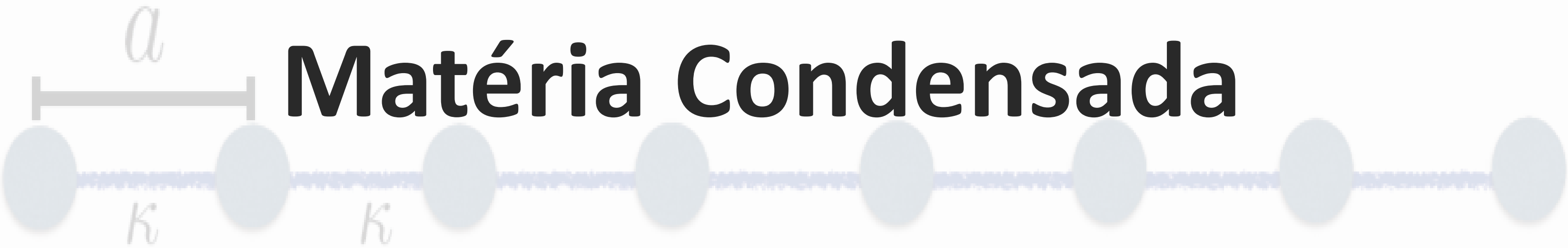
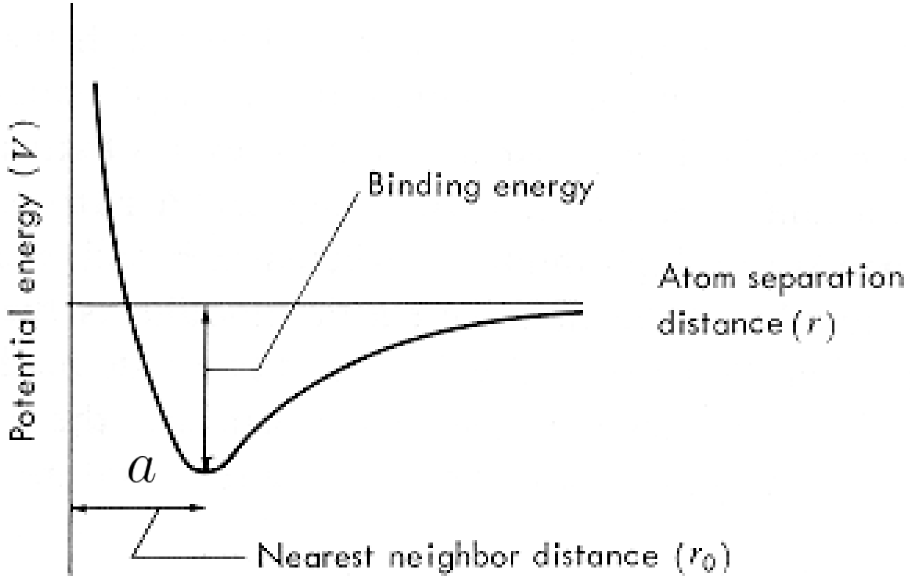
Matéria Condensada



Vibrações cristalinas

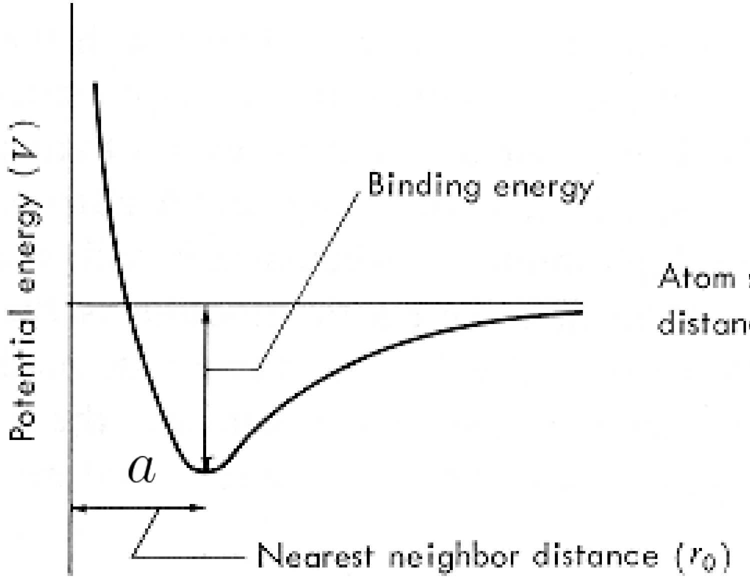
Introdução

- Coesão cristalina



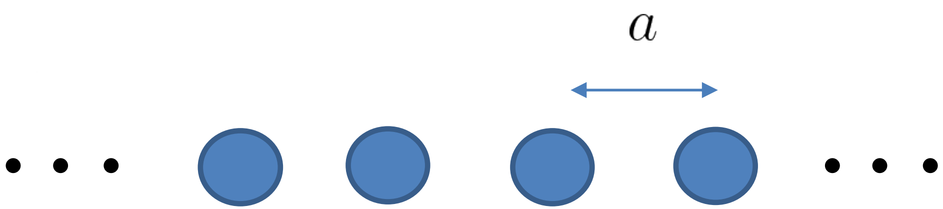
Introdução

- Coesão cristalina

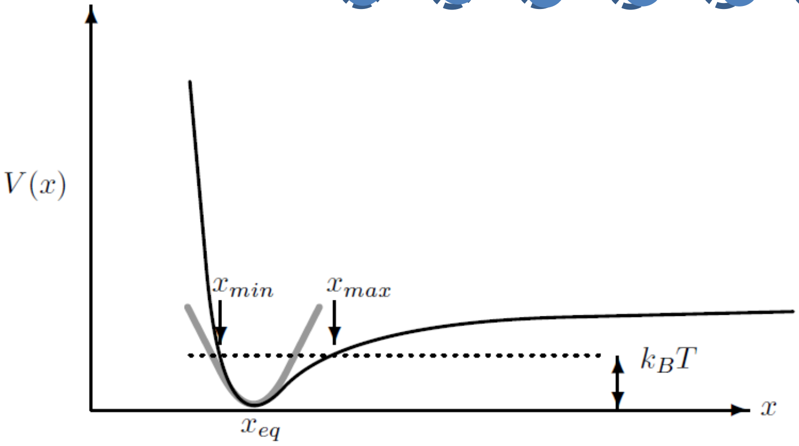


$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 - \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$-\sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|},$$



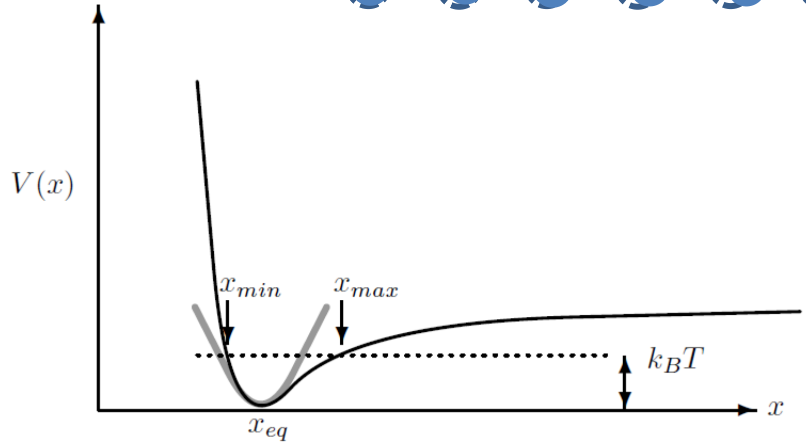
Aproximação Harmônica

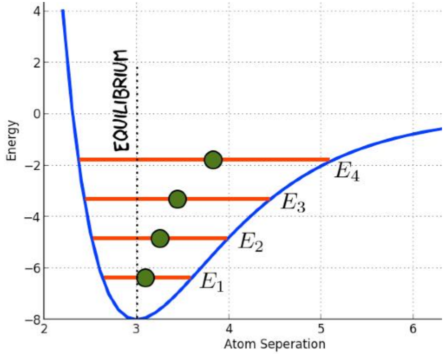


$$V(x) \approx V(x_{eq}) + \frac{\kappa}{2}(x - x_{eq})^2$$

$$-\kappa(\delta x_{eq}) = F$$

Aproximação Harmônica





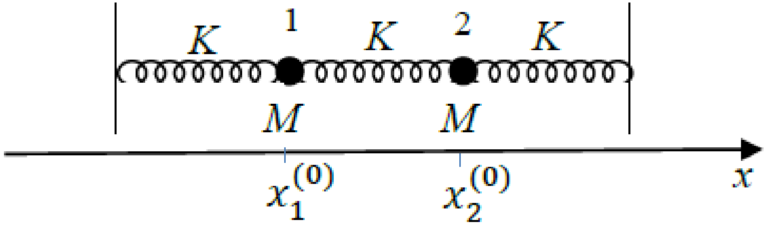
$$V(x) \approx V(x_{eq}) + \frac{\kappa}{2}(x - x_{eq})^2$$

$$-\kappa(\delta x_{eq}) = F$$

$$V(x) \approx V(x_{eq}) + \frac{\kappa}{2}(x - x_{eq})^2$$

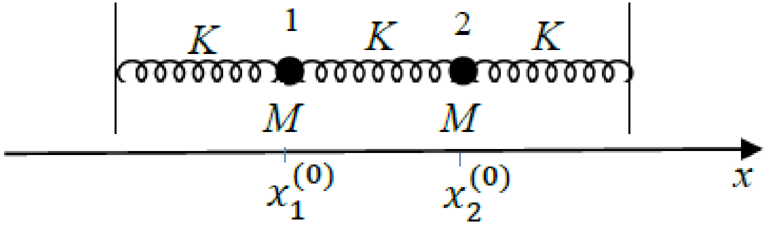
$$-\frac{\kappa_3}{3!}(x - x_{eq})^3 + \ldots .$$

Aproximação Harmônica



$$E = \frac{1}{2} M \dot{u}_1^2 + \frac{1}{2} M \dot{u}_2^2 + \frac{1}{2} K [u_1^2 + (u_1 - u_2)^2 + u_2^2].$$

Aproximação Harmônica



$$E = \frac{1}{2}M\dot{u}_1^2 + \frac{1}{2}M\dot{u}_2^2 + \frac{1}{2}K[u_1^2 + (u_1 - u_2)^2 + u_2^2].$$

$$\begin{cases} F_1 = -Ku_1 - K(u_1 - u_2) = -2Ku_1 + Ku_2 \\ F_2 = -Ku_2 - K(u_2 - u_1) = Ku_1 - 2Ku_2 \end{cases}$$

$$\boldsymbol{F} = -\boldsymbol{\Phi} \cdot \boldsymbol{u}$$

$$\boldsymbol{\Phi} = \begin{bmatrix} 2K & -K \\ -K & 2K \end{bmatrix} = -\begin{bmatrix} \left.\frac{\partial F_1}{\partial u_1}\right|_0 & \left.\frac{\partial F_1}{\partial u_2}\right|_0 \\ \left.\frac{\partial F_2}{\partial u_1}\right|_0 & \left.\frac{\partial F_2}{\partial u_2}\right|_0 \end{bmatrix} = \begin{bmatrix} \left.\frac{\partial^2 U}{\partial u_1 \partial u_1}\right|_0 & \left.\frac{\partial^2 U}{\partial u_1 \partial u_2}\right|_0 \\ \left.\frac{\partial^2 U}{\partial u_2 \partial u_1}\right|_0 & \left.\frac{\partial^2 U}{\partial u_2 \partial u_2}\right|_0 \end{bmatrix}$$

$$E = \frac{1}{2}\mathbf{u} \cdot \mathbf{\Phi} \cdot \mathbf{u}$$

Matriz de constantes de forças

$$q_1 = \frac{u_1 + u_2}{\sqrt{2}};\ q_2 = \frac{u_1 - u_2}{\sqrt{2}}$$

$$E = \left[\tfrac{1}{2} M \dot{q}_1^2 + \tfrac{1}{2} M \omega_1^2 q_1^2\right] + \left[\tfrac{1}{2} M \dot{q}_2^2 + \tfrac{1}{2} M \omega_2^2 q_2^2\right]$$

$$\omega_1 = \sqrt{K/M} \qquad \omega_2 = \sqrt{3K/M}$$

$$q_1 = \frac{u_1+u_2}{\sqrt{2}}; \; q_2 = \frac{u_1-u_2}{\sqrt{2}} \qquad E = \left[\tfrac{1}{2}M\dot{q}_1^2 + \tfrac{1}{2}M\omega_1^2 q_1^2\right] + \left[\tfrac{1}{2}M\dot{q}_2^2 + \tfrac{1}{2}M\omega_2^2 q_2^2\right]$$

$$\omega_1 = \sqrt{K/M} \qquad \omega_2 = \sqrt{3K/M}$$

Como descrever um problema com N átomos?

$$q_1 = \frac{u_1 + u_2}{\sqrt{2}};\ q_2 = \frac{u_1 - u_2}{\sqrt{2}}$$

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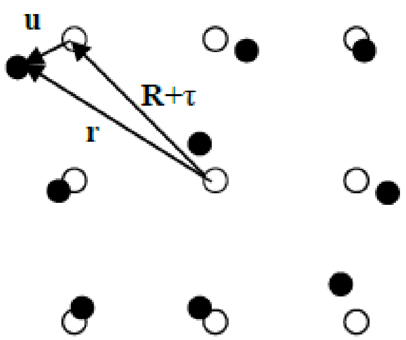
Como descrever um problema com N átomos?



$$\mathbf{r} = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_\mu \\ \vdots \\ r_{3N} \end{bmatrix}; \quad \mathbf{r}^0 = \begin{bmatrix} r_1^0 \\ r_2^0 \\ \vdots \\ r_\mu^0 \\ \vdots \\ r_{3N}^0 \end{bmatrix}; \quad \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_\mu \\ \vdots \\ u_{3N} \end{bmatrix}$$

0

$$U(\mathbf{r}) = U(\mathbf{r}^0 + \mathbf{u}) = U(\mathbf{r}^0) + (\mathbf{u}\cdot\nabla)U\big|_0 + \tfrac{1}{2}(\mathbf{u}\cdot\nabla)^2 U\big|_0 + \dots$$

0

$$U(\mathbf{r}) = U(\mathbf{r}^0 + \mathbf{u}) = U(\mathbf{r}^0) + (\mathbf{u}\cdot\nabla)U\big|_0 + \tfrac{1}{2}(\mathbf{u}\cdot\nabla)^2 U\big|_0 + \dots$$

$$\tfrac{1}{2}(\mathbf{u}\cdot\nabla)^2 U\big|_0 = \frac{1}{2}\left(u_1\frac{\partial}{\partial u_1} + \cdots + u_{3N}\frac{\partial}{\partial u_{3N}}\right)\left(u_1\frac{\partial}{\partial u_1} + \cdots + u_{3N}\frac{\partial}{\partial u_{3N}}\right)U\Big|_0 =$$

$$= \frac{1}{2}\sum_{\substack{\mu=1,\cdots,3N\\ \nu=1,\cdots,3N}} u_\mu \left(\frac{\partial^2 U}{\partial u_\mu \partial u_\nu}\right)\Bigg|_0 u_\nu$$

0

$$U(\mathbf{r}) = U(\mathbf{r}^0 + \mathbf{u}) = U(\mathbf{r}^0) + (\mathbf{u}\cdot\nabla)U\big|_0 + \tfrac{1}{2}(\mathbf{u}\cdot\nabla)^2 U\big|_0 + \dots$$

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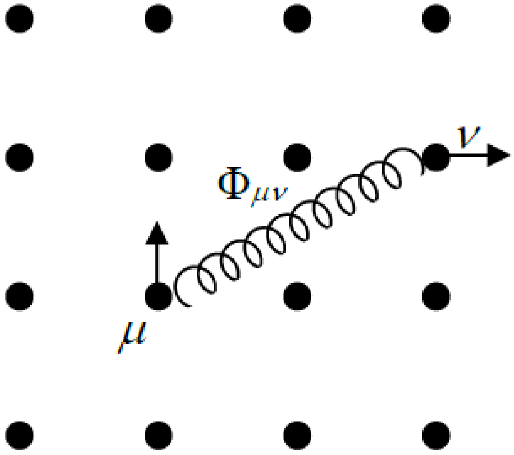
$$= \frac{1}{2}\sum_{\substack{\mu=1,\cdots,3N\\ \nu=1,\cdots,3N}} u_\mu \left(\frac{\partial^2 U}{\partial u_\mu \partial u_\nu}\right)\Bigg|_0 u_\nu$$

$$U = U_0 + \tfrac{1}{2}\mathbf{u}\cdot\mathbf{\Phi}\cdot\mathbf{u}$$

$$\mathbf{\Phi} = \begin{bmatrix} \left.\frac{\partial^2 U}{\partial u_1 \partial u_1}\right|_0 & \cdots & \left.\frac{\partial^2 U}{\partial u_1 \partial u_{3N}}\right|_0 \\ \vdots & \ddots & \vdots \\ \left.\frac{\partial^2 U}{\partial u_{3N} \partial u_1}\right|_0 & \cdots & \left.\frac{\partial^2 U}{\partial u_{3N} \partial u_{3N}}\right|_0 \end{bmatrix}$$

Matriz de constantes de forças

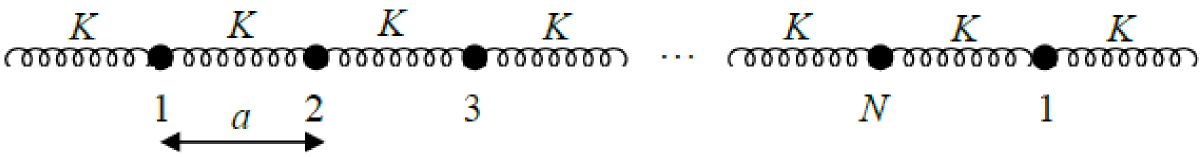
$$\mathbf{F} = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_\mu \\ \vdots \\ F_{3N} \end{bmatrix} = \frac{-\partial U}{\partial \mathbf{u}} = -\mathbf{\Phi} \cdot \mathbf{u}$$



1. A matriz de constante de forças é simétrica: $\Phi_{\mu\nu} = \Phi_{\nu\mu}$

2. $\sum_{\mu} \Phi_{\mu 1} = 0$

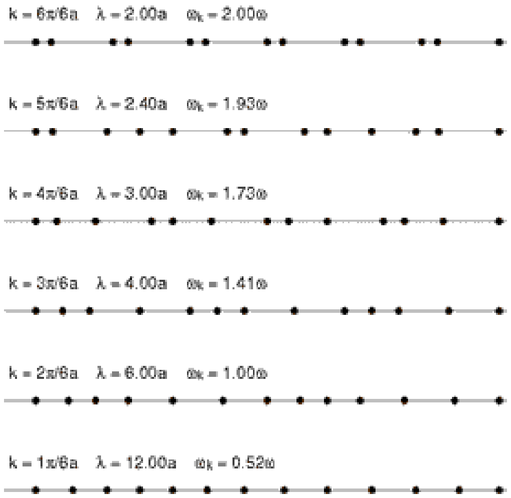
Dificuldades: Diagonalizar a matriz de constante de forças pode ser desafiador.



$$\mathbf{\Phi} = \begin{bmatrix} 2K & -K & 0 & 0 & \cdots & 0 & -K \\ -K & 2K & -K & 0 & \cdots & 0 & 0 \\ 0 & -K & 2K & -K & \cdots & 0 & 0 \\ 0 & 0 & -K & 2K & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & -K & 0 \\ 0 & 0 & 0 & 0 & 0 & 2K & -K \\ -K & 0 & 0 & 0 & 0 & -K & 2K \end{bmatrix}.$$

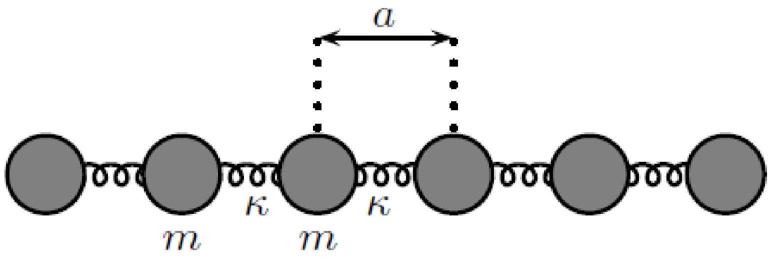
Modos Normais de Vibração

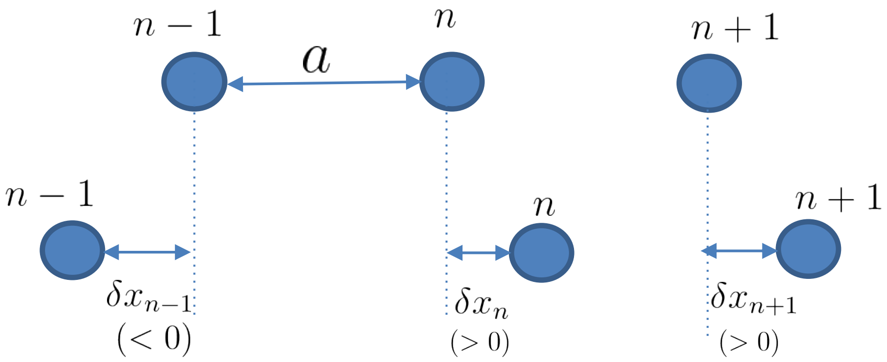
- Os modos normais são excitações **coletivas** nas quais todos os átomos oscilam com a mesma freqüência.



https://en.wikipedia.org/wiki/Phonon

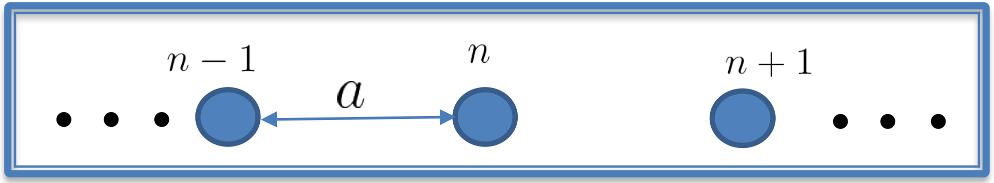
Modos Normais de Vibração





$$m\frac{d^2x_n}{dt^2} = \kappa(\delta x_{n+1} - \delta x_n) - \kappa(\delta x_n - \delta x_{n-1})$$

Estudo dos Modos Normais



$$m\frac{d^2x_n}{dt^2} = \kappa(\delta x_{n+1} - \delta x_n) - \kappa(\delta x_n - \delta x_{n-1})$$

– Buscaremos soluções para os modos normais a partir da *ansatz*

$$\delta x_n = Ae^{i\omega t - ikx_n^{eq}} = Ae^{i(\omega t - nka)}$$

$$\delta x_0 = Ae^{i\omega t} \quad \delta x_1 = Ae^{i\omega t}e^{-ika} \quad \delta x_2 = Ae^{i\omega t}e^{-2ika}$$

$$\delta x_n = Ae^{i(\omega t - nka)} \quad \Rightarrow \quad m\frac{d^2 x_n}{dt^2} = \kappa(\delta x_{n+1} - \delta x_n) - \kappa(\delta x_n - \delta x_{n-1})$$

$$-m\omega^2 Ae^{i\omega t - ikna} = \kappa Ae^{i\omega t}\left[e^{-ika(n+1)} + e^{-ika(n-1)} - 2e^{-ikan}\right]$$

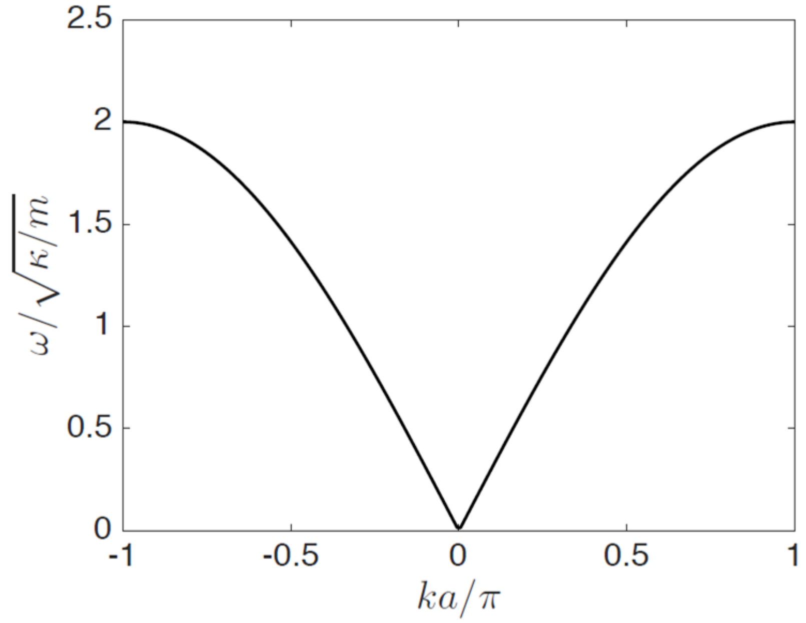
$$\delta x_n = Ae^{i(\omega t - nka)} \quad \Rightarrow \quad m\frac{d^2 x_n}{dt^2} = \kappa(\delta x_{n+1} - \delta x_n) - \kappa(\delta x_n - \delta x_{n-1})$$

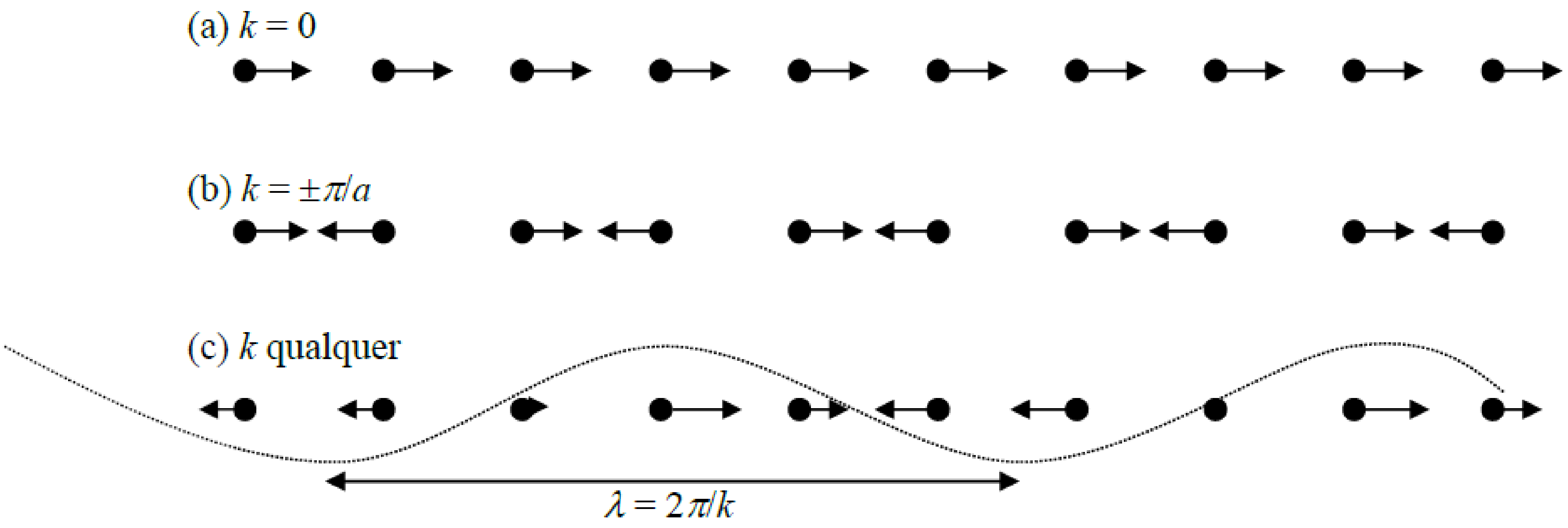
$$-m\omega^2 Ae^{i\omega t - ikna} = \kappa Ae^{i\omega t}\left[e^{-ika(n+1)} + e^{-ika(n-1)} - 2e^{-ikan}\right]$$

$$m\omega^2 = 2\kappa[1 - \cos(ka)] = 4\kappa\sin^2(ka/2)$$

Relação de dispersão

$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$





(a) $k = 0$
(b) $k = \pm\pi/a$
(c) k qualquer
$\lambda = 2\pi/k$

Velocidade do som

$$v = \sqrt{\frac{B}{\rho}} = \sqrt{\frac{1}{\rho\beta}}$$

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Compressibilidade

$$\beta = -\frac{1}{V}\frac{\partial V}{\partial P}$$

$$\beta = -\frac{1}{L}\frac{\partial L}{\partial F} = \frac{1}{\kappa\, x_{eq}} = \frac{1}{\kappa\, a}$$

$$v = \sqrt{\frac{\kappa a^2}{m}}.$$

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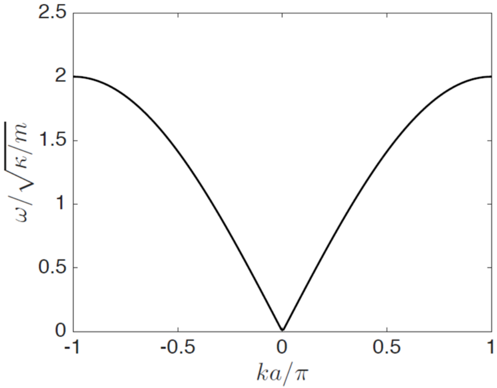
Velocidade de grupo



$$v_{group} = d\omega/dk$$

Velocidade do som

$$v = \sqrt{\frac{B}{\rho}} = \sqrt{\frac{1}{\rho\beta}}$$

Compressibilidade

$$\beta = -\frac{1}{V}\frac{\partial V}{\partial P}$$

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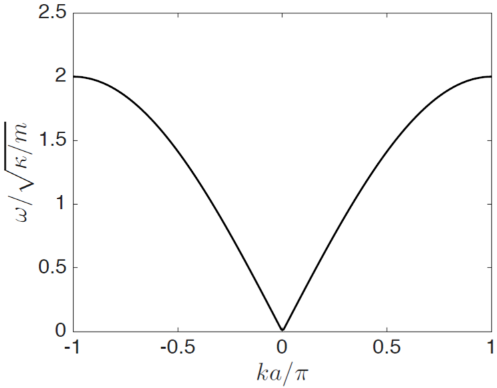
Velocidade de grupo



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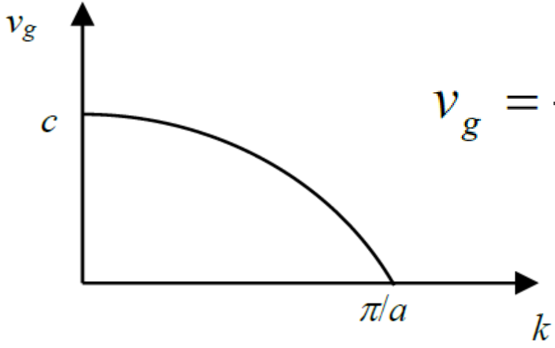
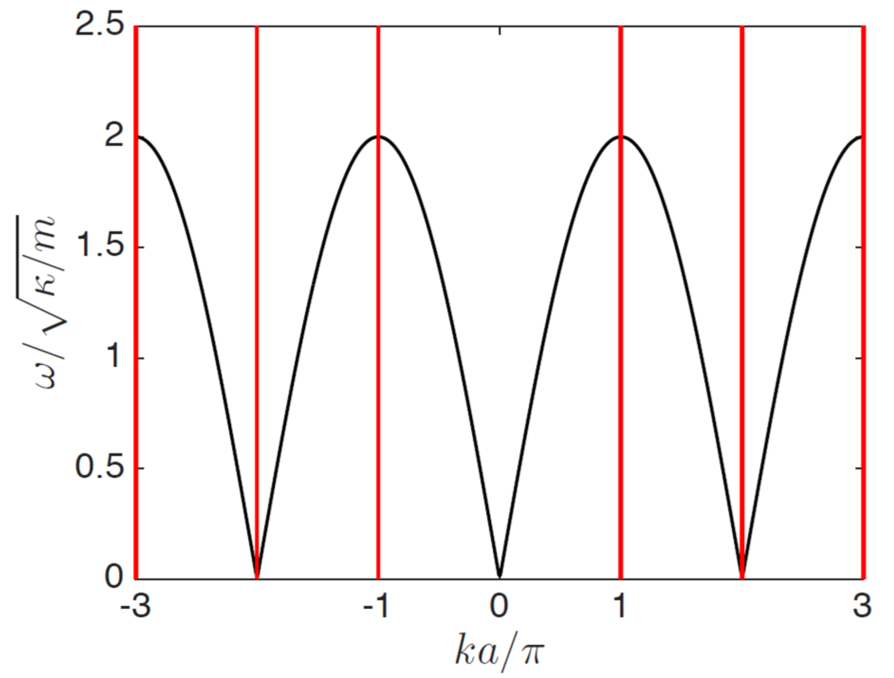


$$v_g = \frac{d\omega}{dk} = a\sqrt{\frac{K}{M}}\cos\frac{ka}{2}$$

1ª Zona de Brillouin



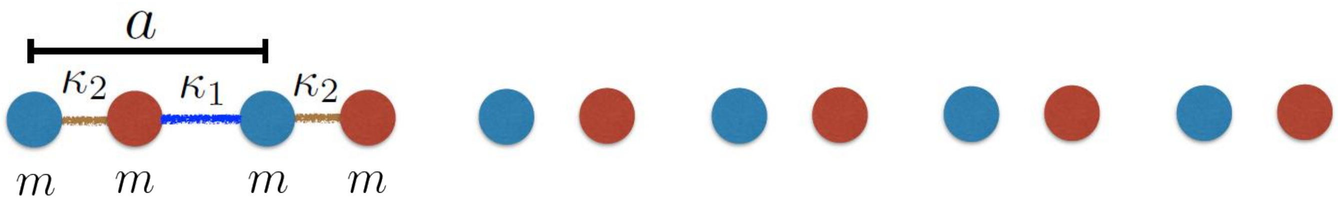
$$\mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 + \frac{n_3}{N_3}\mathbf{b}_3$$

$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\mathrm{sen}\left(\frac{ka}{2}\right)\right|$$

$$k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

Cadeia diatômica

- Seja uma cadeia formada por dois tipos de átomos (ou ligações).



Cadeia diatômica

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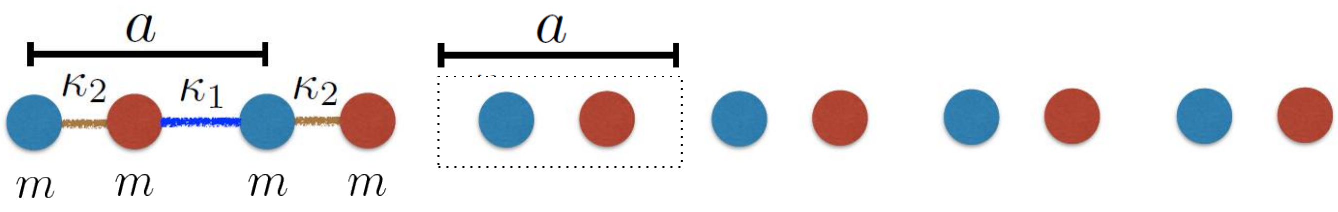
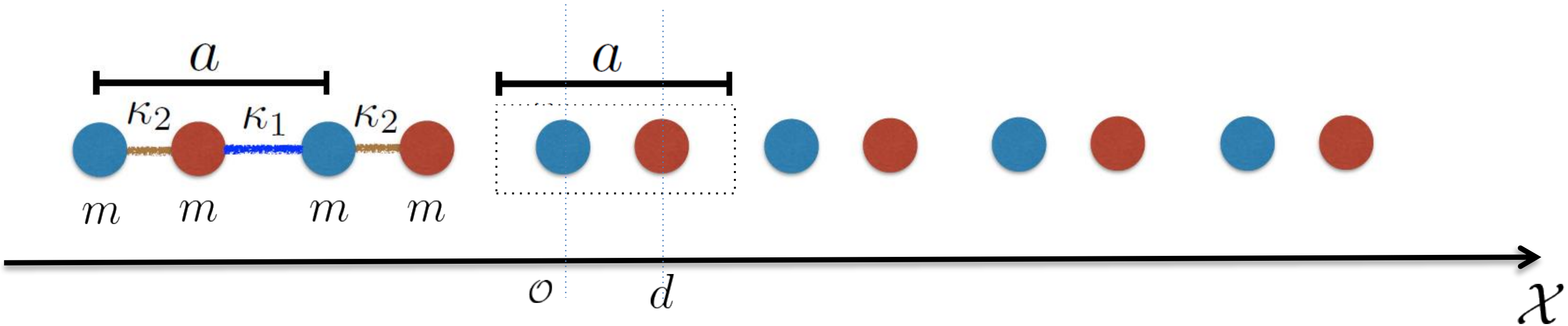


- Definição de célula unitária.

Cadeia diatômica

- Seja uma cadeia formada por dois tipos de átomos (ou ligações).



- Definição de célula unitária.
- Base: $0, d$

Cadeia diatômica

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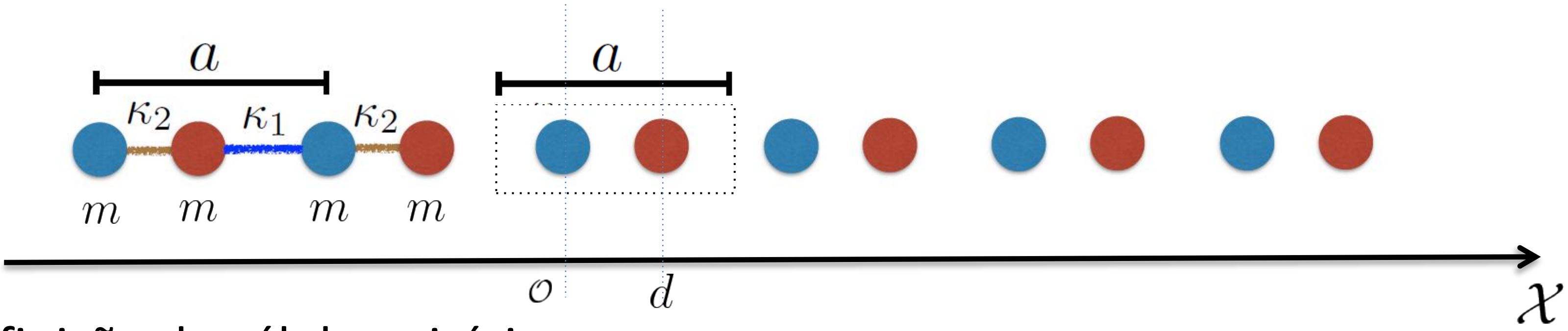
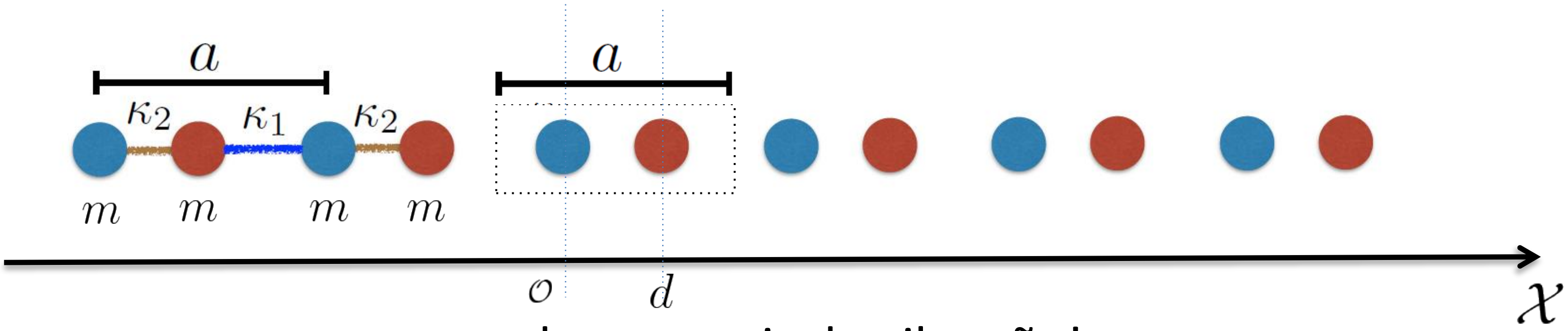


- Definição de célula unitária.
- Base: $0, d$
- 1ª Zona de Brillouin: $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$

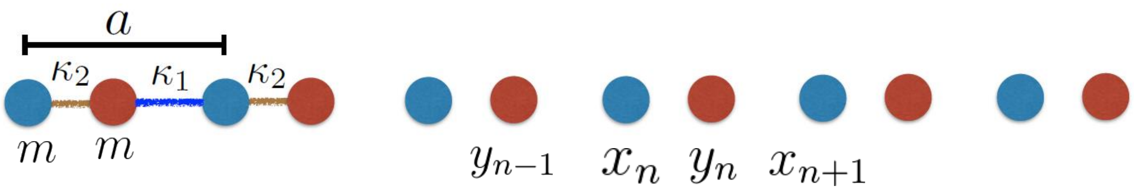
Cadeia diatômica

- Seja uma cadeia formada por dois tipos de átomos (ou ligações).



- Devemos encontrar os modos normais de vibração!

Cadeia diatômica



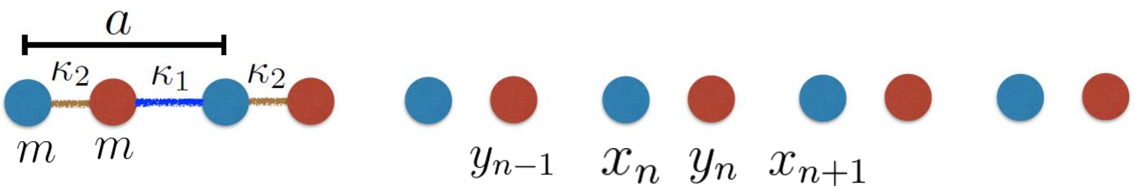
- As equações de movimento neste caso são:

$$m\frac{d^2(\delta x_n)}{dt^2} = \kappa_2(\delta y_n - \delta x_n) + \kappa_1(\delta y_{n-1} - \delta x_n)$$

$$m\frac{d^2(\delta y_n)}{dt^2} = \kappa_1(\delta x_{n+1} - \delta y_n) + \kappa_2(\delta x_n - \delta y_n)$$

$$(n = 1, \cdots, N)$$

Cadeia diatômica



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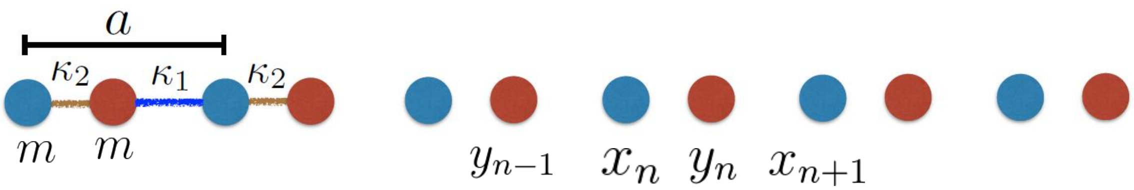
$$(n = 1, \cdots, N)$$

- Ansätze:

$$\delta x_n = A_x e^{-ikna+i\omega t}$$

Cadeia diatômica



- As equações de movimento neste caso são:

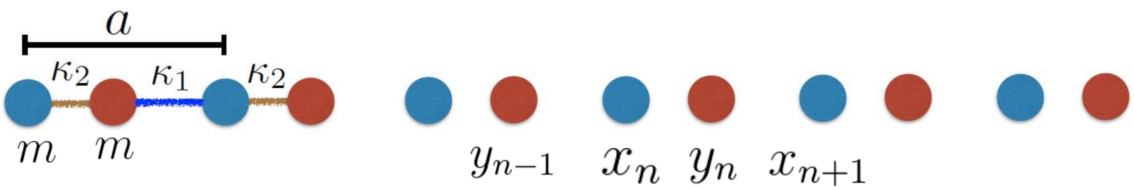
$$
\begin{aligned}
m\frac{d^2\left(\delta x_n\right)}{dt^2} &= \kappa_2\left(\delta y_n - \delta x_n\right) + \kappa_1\left(\delta y_{n-1} - \delta x_n\right) \\
m\frac{d^2\left(\delta y_n\right)}{dt^2} &= \kappa_1\left(\delta x_{n+1} - \delta y_n\right) + \kappa_2\left(\delta x_n - \delta y_n\right)
\end{aligned}
$$

$$(n = 1, \cdots, N)$$

- Ansätze:

$$
\begin{aligned}
\delta x_n &= A_x e^{-ikna+i\omega t} \\
\delta y_n &= A_y e^{-ikna+i\omega t}
\end{aligned}
$$

Cadeia diatômica



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\begin{aligned}
m\frac{d^2(\delta x_n)}{dt^2} &= \kappa_2(\delta y_n - \delta x_n) + \kappa_1(\delta y_{n-1} - \delta x_n) \\
m\frac{d^2(\delta y_n)}{dt^2} &= \kappa_1(\delta x_{n+1} - \delta y_n) + \kappa_2(\delta x_n - \delta y_n)
\end{aligned}
$$

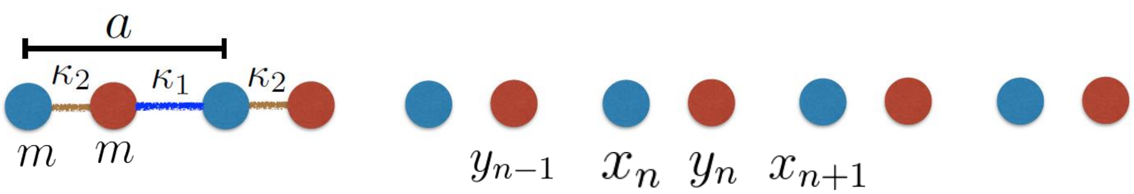
$$(n = 1, \cdots, N)$$

- Ansätze:

$$
\begin{aligned}
\delta x_n &= A_x e^{-ikna+i\omega t} \\
\delta y_n &= A_y e^{-ikna+i\omega t}
\end{aligned}
$$

$$A_x, A_y \in \mathbb{C}$$

Cadeia diatômica



- As equações de movimento neste caso são:

$$\delta x_n = A_x e^{-ikna+i\omega t}$$
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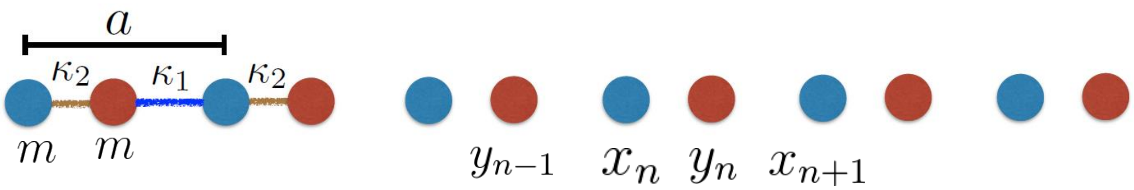
$$m\frac{d^2(\delta x_n)}{dt^2} = \kappa_2(\delta y_n - \delta x_n) + \kappa_1(\delta y_{n-1} - \delta x_n)$$
$$m\frac{d^2(\delta y_n)}{dt^2} = \kappa_1(\delta x_{n+1} - \delta y_n) + \kappa_2(\delta x_n - \delta y_n)$$

Cadeia diatômica



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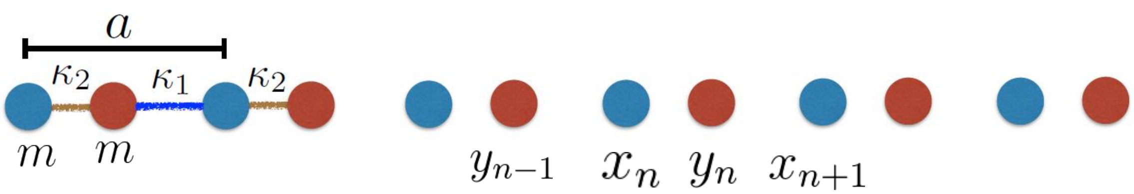
- Após alguma álgebra:

$$m\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} \kappa_1 + \kappa_2 & -\kappa_2 - \kappa_1 e^{ika} \\ -\kappa_2 - \kappa_1 e^{-ika} & \kappa_1 + \kappa_2 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

Cadeia diatômica



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Matriz 2 x 2 !!

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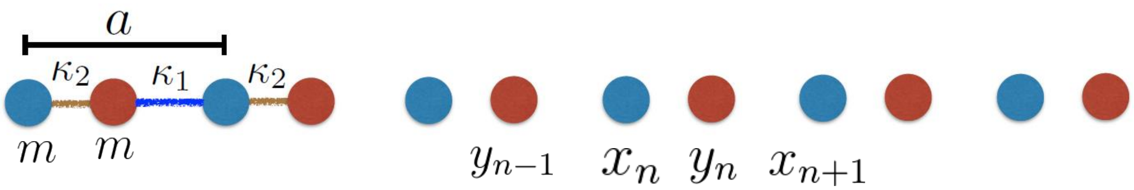

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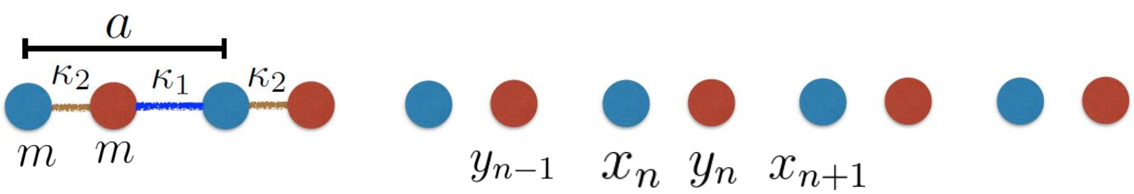
- Após alguma álgebra:

Matriz 2 x 2 !!

Para cada k há 2 ω's!!

$$m\omega^2\begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} \kappa_1+\kappa_2 & -\kappa_2-\kappa_1 e^{ika} \\ -\kappa_2-\kappa_1 e^{-ika} & \kappa_1+\kappa_2 \end{pmatrix}\begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

Cadeia diatômica

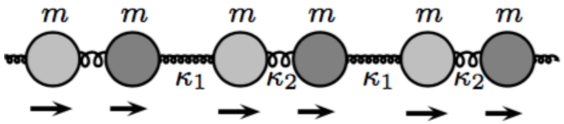


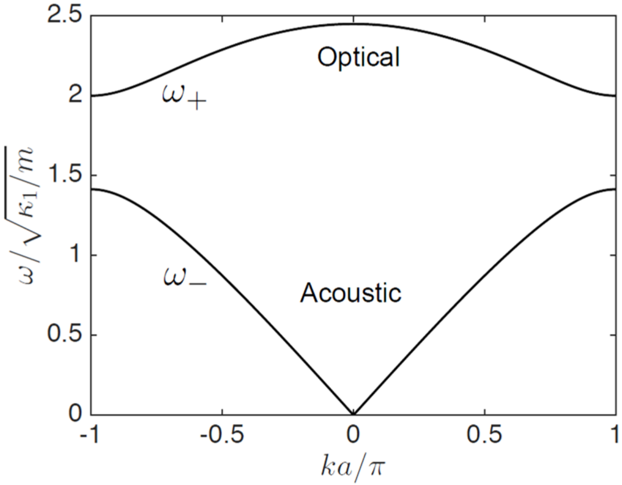
- Encontrando os autovalores da matriz anterior obtemos

$$\omega_\pm = \sqrt{\frac{\kappa_1 + \kappa_2}{m} \pm \frac{1}{m}\sqrt{\kappa_1^2 + \kappa_2^2 + 2\kappa_1\kappa_2\cos(ka)}}$$

- Autovetores $ka \ll 1$:

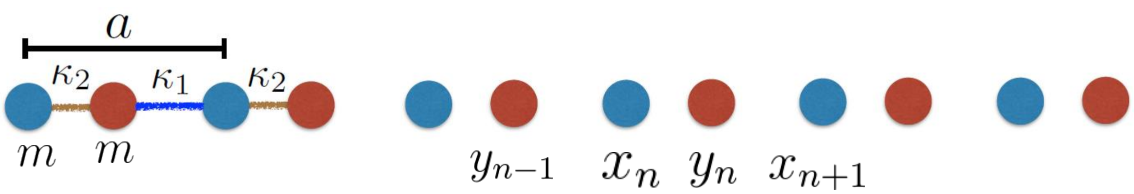
$$\omega_- \rightarrow A_1 = A_2$$





$\kappa_2 = 2\kappa_1$

Cadeia diatômica



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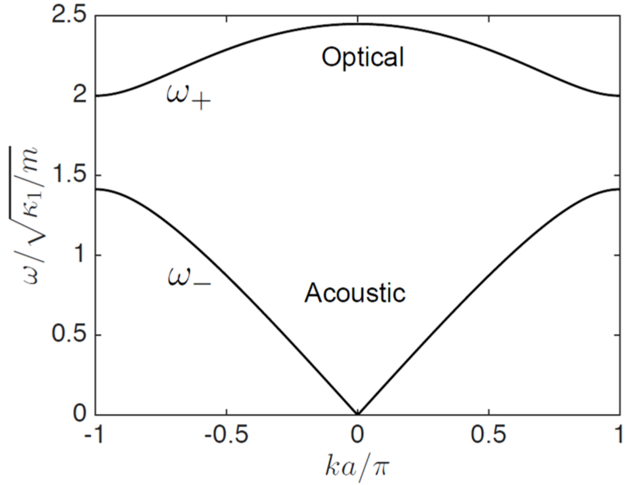
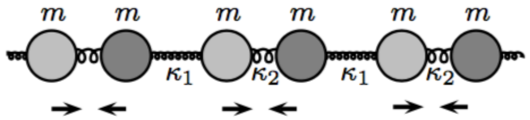


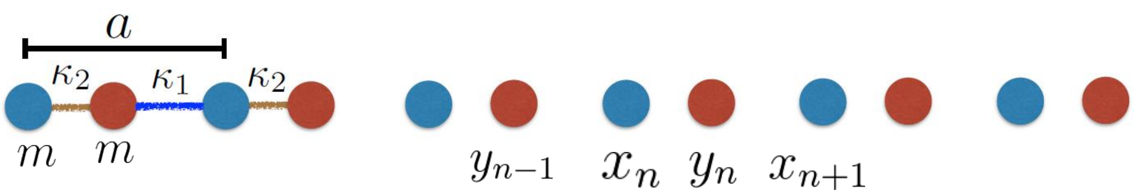
$\kappa_2 = 2\kappa_1$

- Autovetores $ka \ll 1$:

$$\omega_+ \rightarrow A_1 = -A_2$$



Cadeia diatômica



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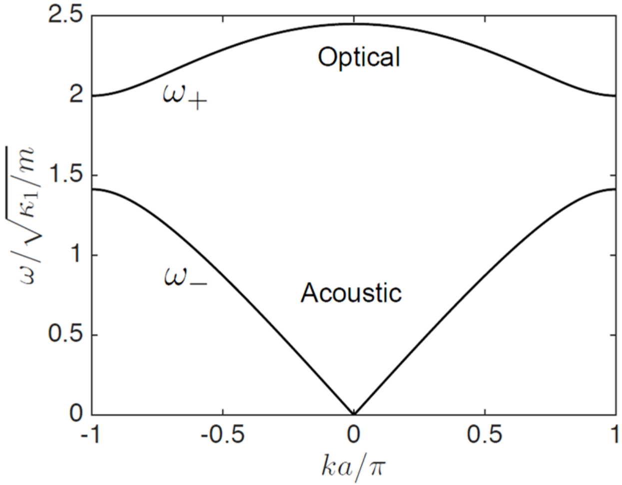


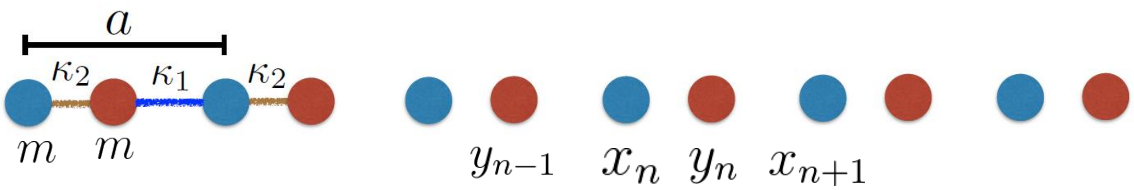
$\kappa_2 = 2\kappa_1$

- Para $ka << 1$:
  - Ramo acústico:

$$\omega_- \approx v_{\rm som} k$$

$$v_{\rm som} = \frac{d\omega_-}{dk} = \sqrt{\frac{a^2\kappa_1\kappa_2}{2m(\kappa_1+\kappa_2)}}$$

Cadeia diatômica



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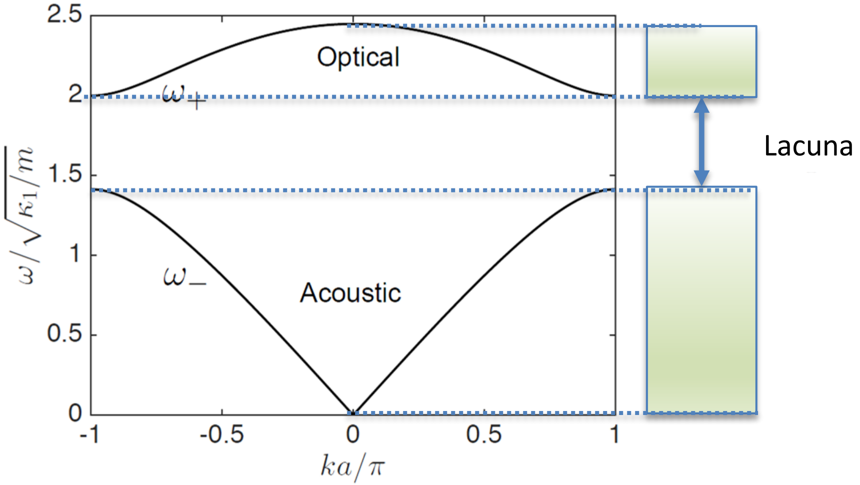

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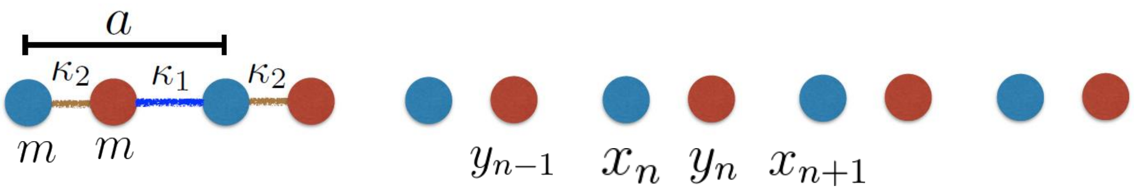
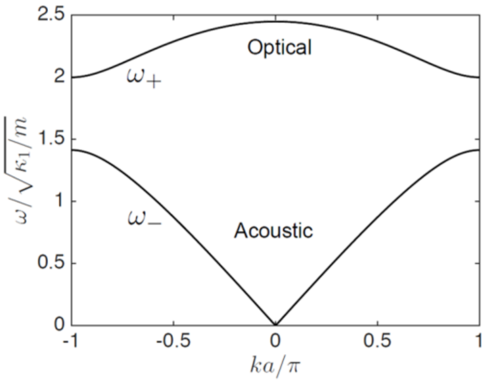
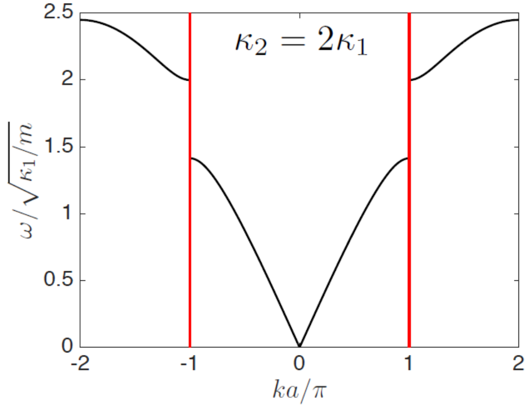


- Outra forma de representar a relação de dispersão:



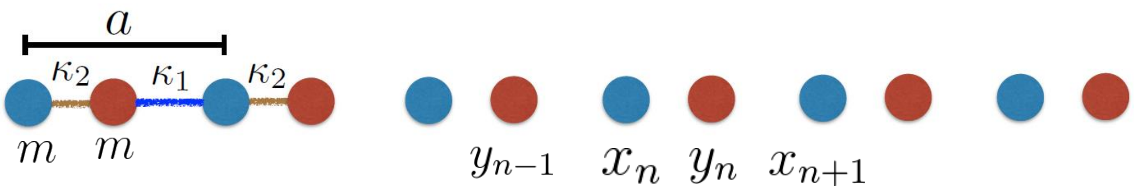
$\kappa_2 = 2\kappa_1$

Zona reduzida

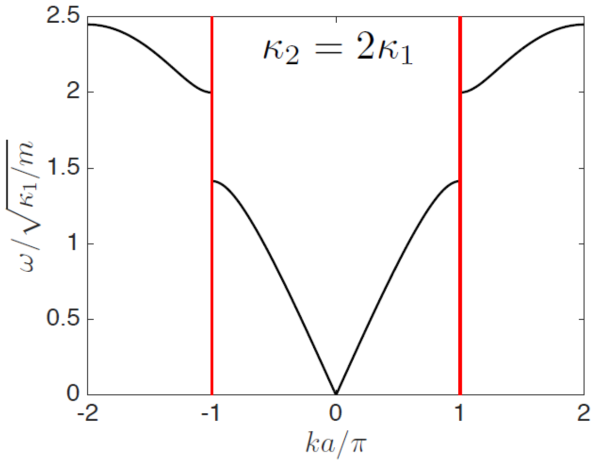


Zona Estendida

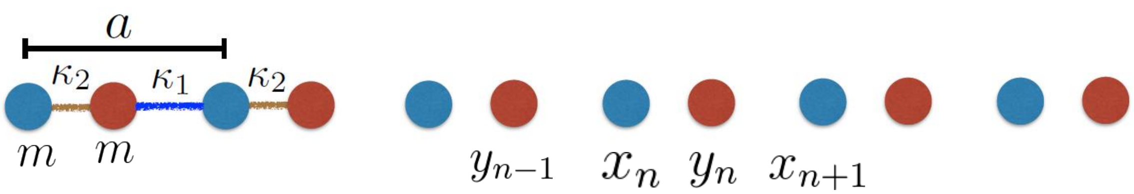
Cadeia diatômica



- Vejamos o que acontece quando $\kappa_2 \to \kappa_1$



Cadeia diatômica



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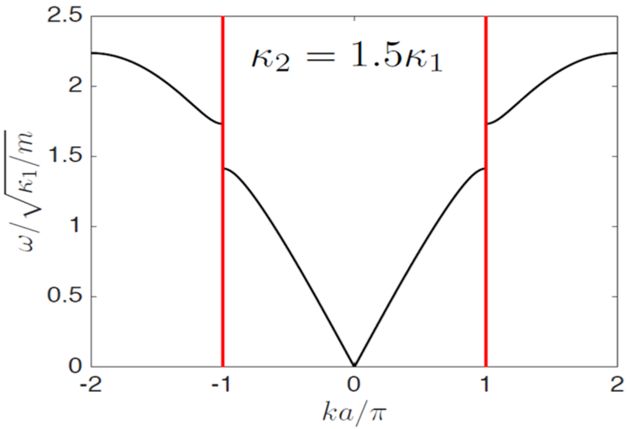

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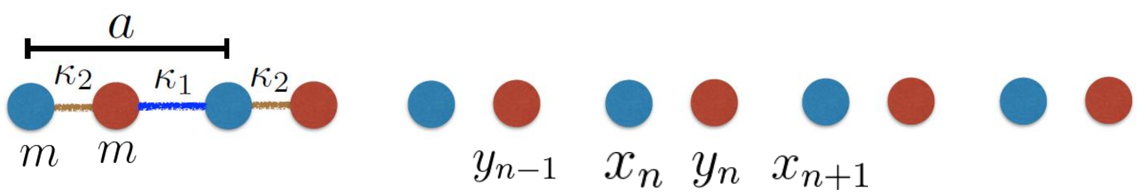

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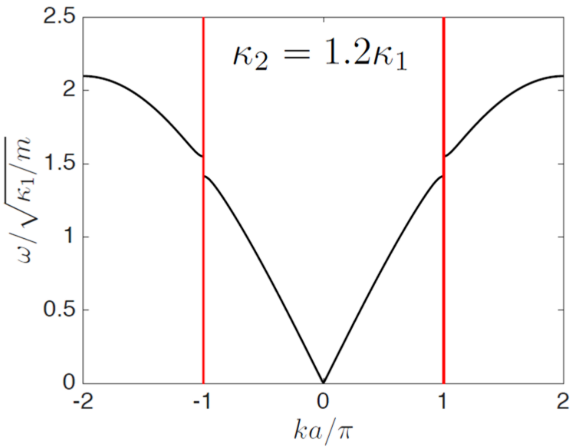
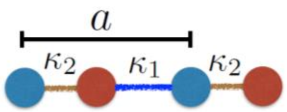
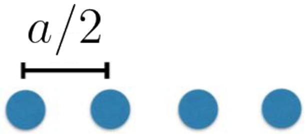


Cadeia diatômica





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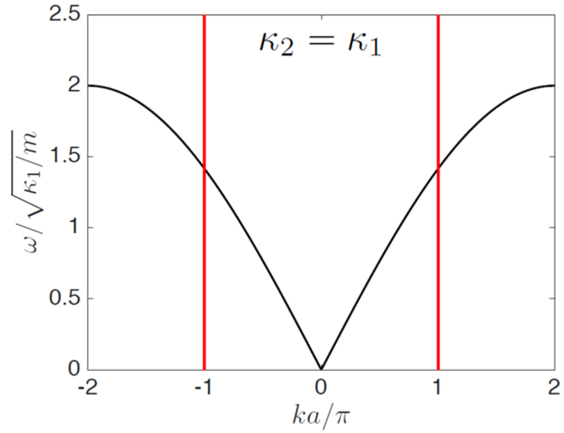
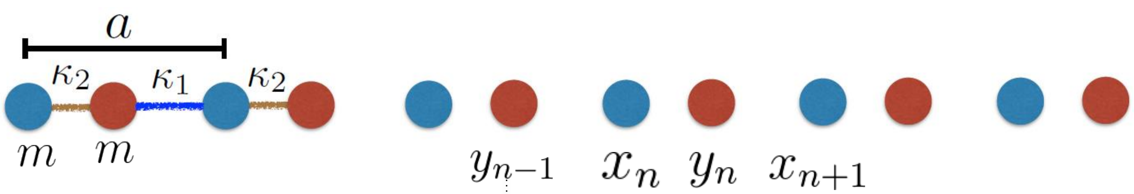
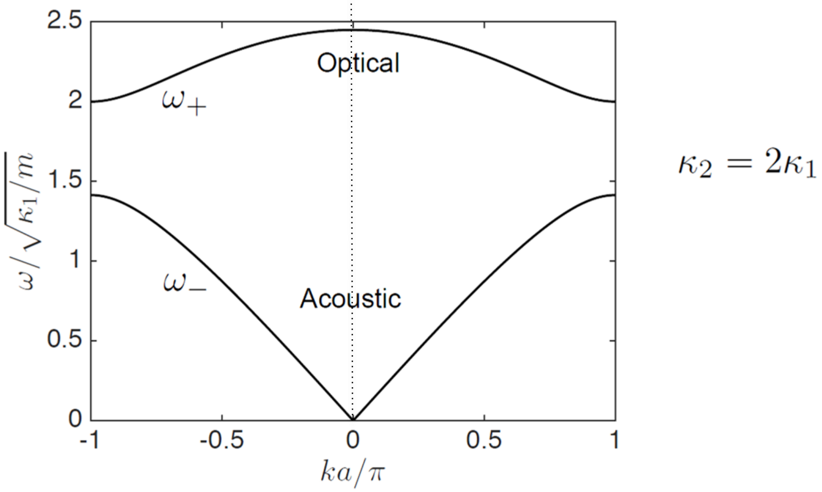


Cadeia diatômica



- O porquê dos nomes:



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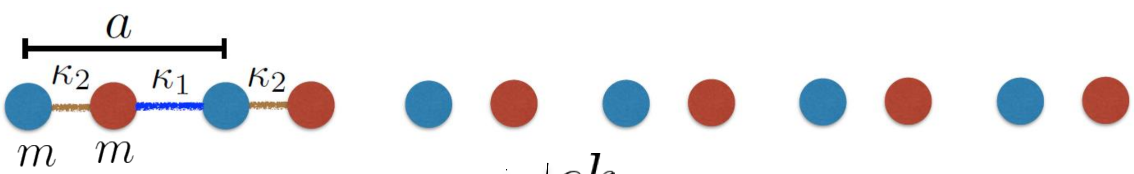

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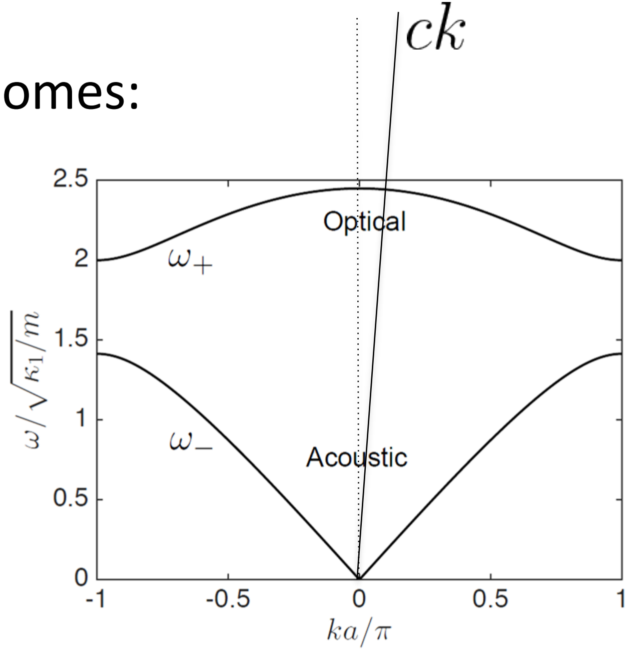
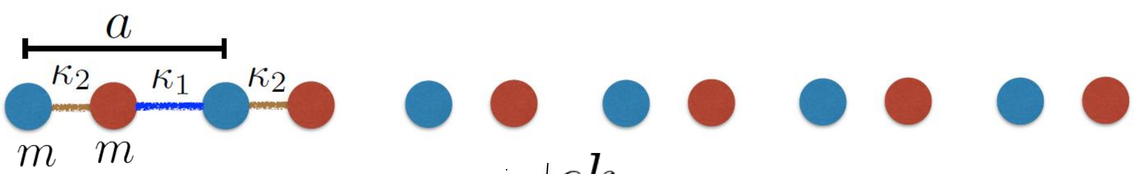


$\kappa_2 = 2\kappa_1$

Cadeia diatômica



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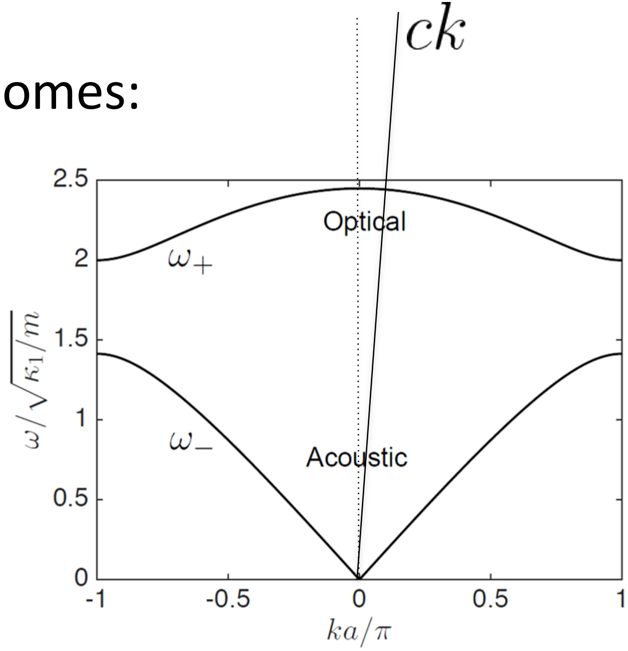
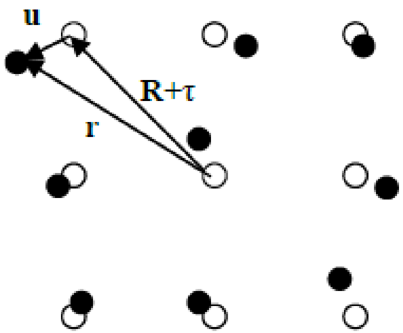


Fônons óticos tem energia da ordem ~ 10^2 meV!

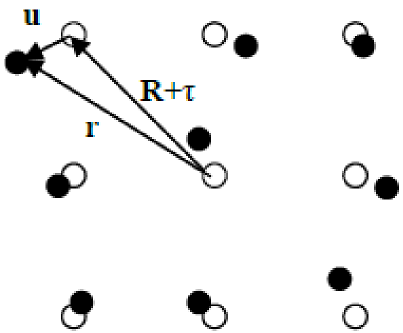
$\kappa_2 = 2\kappa_1$

Como descrever um problema similar com N átomos?



$$\mathbf{u} \equiv \mathbf{u}_{\mathbf{R},\boldsymbol{\tau}}(t) = u_{\mathbf{R},\boldsymbol{\tau},x}(t)\hat{x} + u_{\mathbf{R},\boldsymbol{\tau},y}(t)\hat{y} + u_{\mathbf{R},\boldsymbol{\tau},z}(t)\hat{z}$$

Como descrever um problema similar com N átomos?



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$$\mathbf{u}_{\mathbf{R},\tau}(t) = \frac{1}{\sqrt{M_{\boldsymbol{\tau}}}} \sum_{\mathbf{k}} \hat{\boldsymbol{\varepsilon}}_{\tau}(\mathbf{k}) e^{i[\mathbf{k}\cdot\mathbf{R} - \omega(\mathbf{k})t]}$$

$$\mathbf{q}_{\mathbf{k}}(t) = \frac{1}{\sqrt{M_{\tau}}} \hat{\boldsymbol{\varepsilon}}_{\boldsymbol{\tau}}(\mathbf{k}) e^{i[\mathbf{k}\cdot\mathbf{R} - \omega(\mathbf{k})t]}$$

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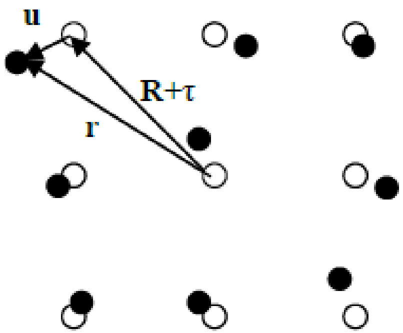

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Notem que o uso de PBC nos leva nos mesmos vetores da rede recíproca do caso eletrônico, que, por sua vez, nos levam nos mesmos vetores k’s da 1ª ZB.

$$\mathbf{u}_{\mathbf{R},\tau} = \mathbf{u}_{\mathbf{R}+N_i\mathbf{a}_i,\tau} \quad \Rightarrow \quad \mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 + \frac{n_3}{N_3}\mathbf{b}_3$$

$$M_{\boldsymbol{\tau}}\ddot{u}_{\mathbf{R},\boldsymbol{\tau},\alpha} = F_{\mathbf{R},\boldsymbol{\tau},\alpha} = -(\boldsymbol{\Phi}\cdot\mathbf{u})_{\mathbf{R},\boldsymbol{\tau},\alpha} = -\sum_{\mathbf{R}',\boldsymbol{\tau}',\alpha'}\Phi_{\mathbf{R}\boldsymbol{\tau}\alpha,\mathbf{R}'\boldsymbol{\tau}'\alpha'}u_{\mathbf{R}',\boldsymbol{\tau}',\alpha'}$$

$$M_{\boldsymbol{\tau}} \ddot{u}_{\mathbf{R},\boldsymbol{\tau},\alpha} = F_{\mathbf{R},\boldsymbol{\tau},\alpha} = -(\boldsymbol{\Phi} \cdot \mathbf{u})_{\mathbf{R},\boldsymbol{\tau},\alpha} = -\sum_{\mathbf{R}',\boldsymbol{\tau}',\alpha'} \Phi_{\mathbf{R}\boldsymbol{\tau}\alpha,\mathbf{R}'\boldsymbol{\tau}'\alpha'} u_{\mathbf{R}',\boldsymbol{\tau}',\alpha'}$$

$$-M_{\tau}\omega^2 \frac{\varepsilon_{\tau,\alpha}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}}}{\sqrt{M_{\tau}}} = -\sum_{\mathbf{R}',\tau',\alpha'} \frac{\Phi_{\mathbf{R}\tau\alpha,\mathbf{R}'\tau'\alpha'}\varepsilon_{\tau'\alpha'}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}'}}{\sqrt{M_{\tau'}}}$$

$$\Rightarrow$$

$$\omega^2 \varepsilon_{\tau,\alpha}(\mathbf{k}) = \sum_{\tau',\alpha'} \left[\sum_{\mathbf{R}'} \frac{\Phi_{\mathbf{R}\tau\alpha,\mathbf{R}'\tau'\alpha'} e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}}{\sqrt{M_{\tau}M_{\tau'}}} \right] \varepsilon_{\tau'\alpha'}(\mathbf{k})$$

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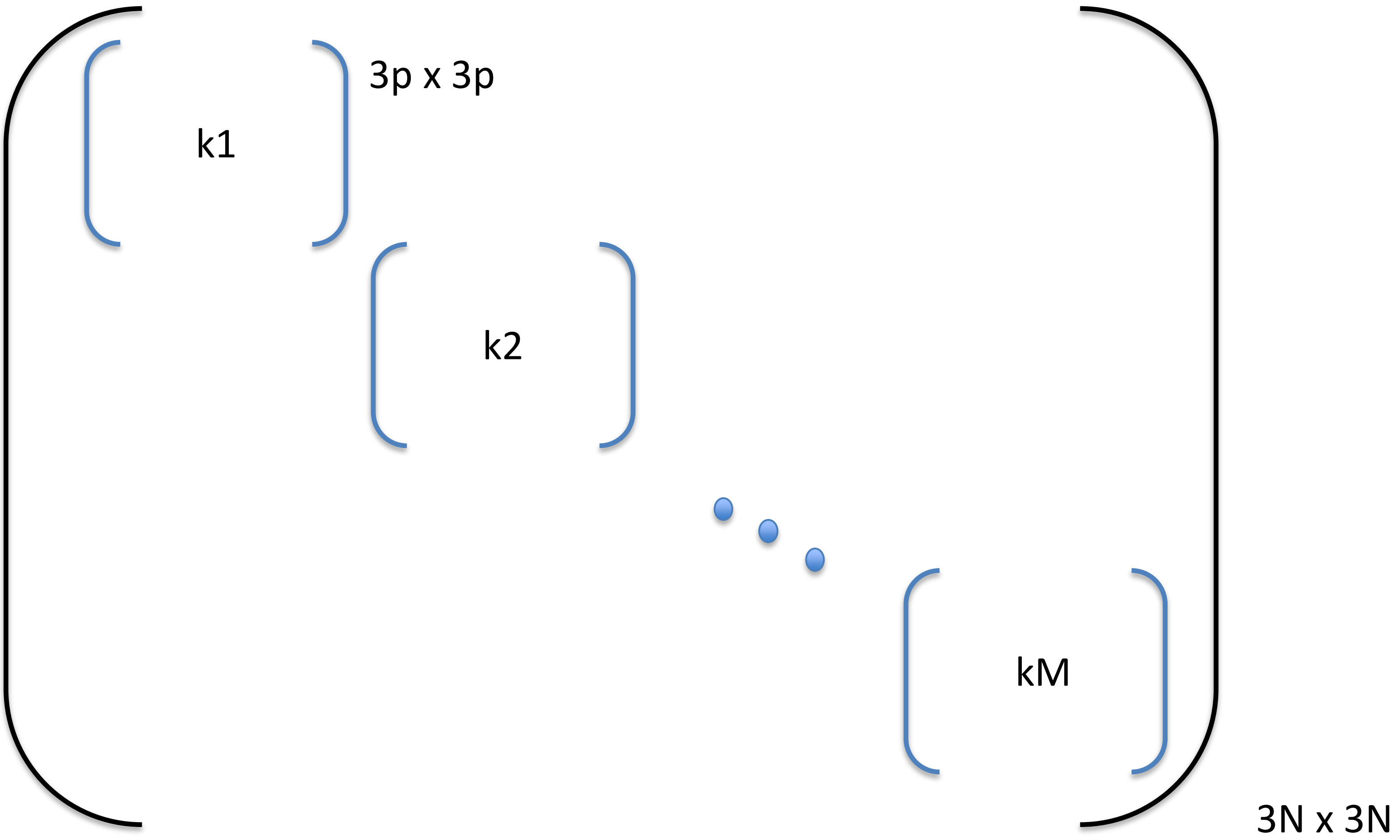
$$\omega^2\varepsilon_{\tau,\alpha}(\mathbf{k}) = \sum_{\tau',\alpha'}\left[\sum_{\mathbf{R}'}\frac{\Phi_{\mathbf{R}\tau\alpha,\mathbf{R}'\tau'\alpha'}e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}}{\sqrt{M_\tau M_{\tau'}}}\right]\varepsilon_{\tau'\alpha'}(\mathbf{k})$$

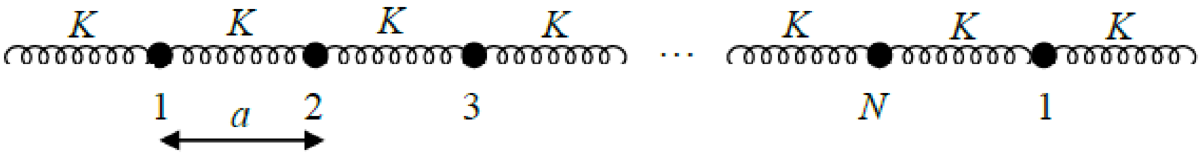
$$\omega^2\varepsilon_i(\mathbf{k}) = \sum_j\left[\sum_{\mathbf{R}'}\frac{\Phi_{\mathbf{R}i,\mathbf{R}'j}e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}}{\sqrt{M_i M_j}}\right]\varepsilon_j(\mathbf{k})$$

$$\begin{cases}\omega^2\hat{\boldsymbol{\varepsilon}}(\mathbf{k}) = \mathbf{D}(\mathbf{k})\cdot\hat{\boldsymbol{\varepsilon}}(\mathbf{k}) \\ D_{ij}(\mathbf{k}) = \dfrac{1}{\sqrt{M_i M_j}}\displaystyle\sum_{\mathbf{R}'}\Phi_{\mathbf{R}i,\mathbf{R}'j}e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}\end{cases}$$

D(k) → matriz dinâmica

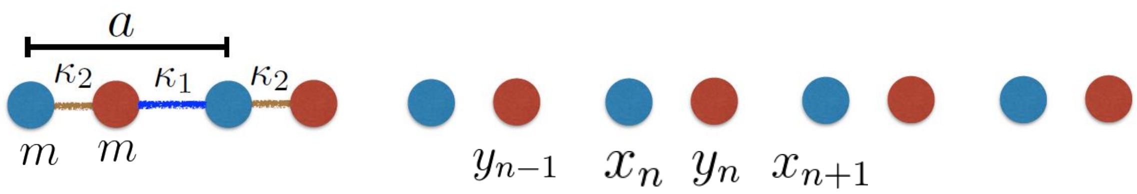
$$i \equiv (\boldsymbol{\tau},\alpha)$$


3p x 3p
k1
k2
kM
3N x 3N

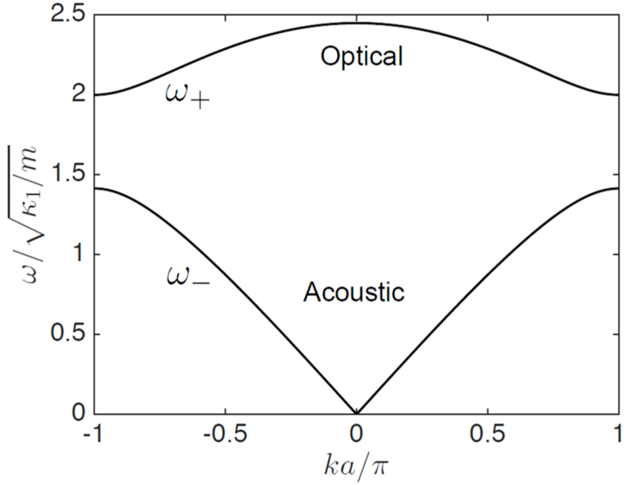


$$\mathbf{\Phi} = \begin{bmatrix} 2K & -K & 0 & 0 & \cdots & 0 & -K \\ -K & 2K & -K & 0 & \cdots & 0 & 0 \\ 0 & -K & 2K & -K & \cdots & 0 & 0 \\ 0 & 0 & -K & 2K & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & -K & 0 \\ 0 & 0 & 0 & 0 & 0 & 2K & -K \\ -K & 0 & 0 & 0 & 0 & -K & 2K \end{bmatrix}.$$

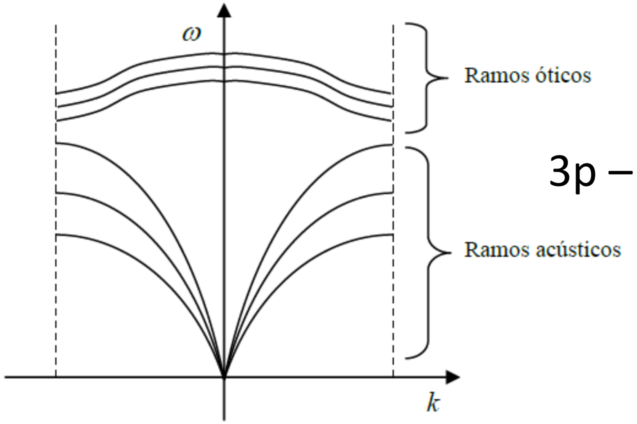
$$D(k) = \frac{4K}{M} \operatorname{sen}^2\left(\frac{ka}{2}\right)$$



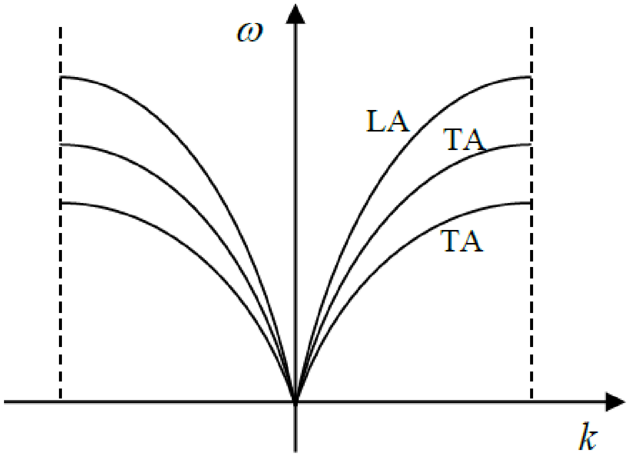
$$D(k) = \frac{1}{m}\begin{pmatrix} \kappa_1+\kappa_2 & -\kappa_2-\kappa_1 e^{ika} \\ -\kappa_2-\kappa_1 e^{-ika} & \kappa_1+\kappa_2 \end{pmatrix}$$



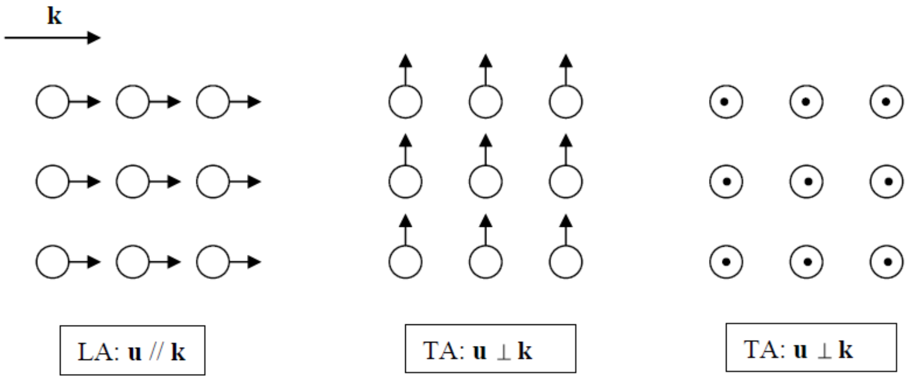
Vibrações em 3D



3p – 3 modos óticos



APENAS 3 modos longitudinais



Calor específico

Calor específico

Contribuição térmica

$$E = \frac{\int \mathrm{d}\Gamma\, \mathcal{H} \mathrm{e}^{-\beta \mathcal{H}}}{\int \mathrm{d}\Gamma\, \mathrm{e}^{-\beta \mathcal{H}}}$$

com

$$\mathrm{d}\Gamma = \prod_{m,\mu} \mathrm{d}\boldsymbol{u}(m,\mu)\, \mathrm{d}\boldsymbol{P}(m,\mu)$$

Calor específico

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$$\mathrm{d}\Gamma = \prod_{m,\mu} \mathrm{d}\boldsymbol{u}(m,\mu)\, \mathrm{d}\boldsymbol{P}(m,\mu)$$

Mudando para modos normais, temos

$$E = \sum_{\boldsymbol{q},\lambda} \frac{\int \mathrm{d}\Gamma_\lambda(\boldsymbol{q})\, \mathcal{H}_\lambda(\boldsymbol{q}) \mathrm{e}^{-\beta\mathcal{H}_\lambda(\boldsymbol{q})}}{\int \mathrm{d}\Gamma_\lambda(\boldsymbol{q})\, \mathrm{e}^{-\beta\mathcal{H}_\lambda(\boldsymbol{q})}}$$

com

$$\mathrm{d}\Gamma = \prod_{\boldsymbol{q},\lambda} \mathrm{d}|Q_\lambda(\boldsymbol{q})|\, \mathrm{d}|P_\lambda(\boldsymbol{q})| \,.$$

$$\mathcal{H}_\lambda(\boldsymbol{q}) = \tfrac{1}{2} \left\{ |P_\lambda(\boldsymbol{q})|^2 + \omega_\lambda^2(\boldsymbol{q}) |Q_\lambda(\boldsymbol{q})|^2 \right\}$$

Calor específico

Contribuição térmica

$$E = \frac{\int \mathrm{d}\Gamma\, \mathcal{H} \mathrm{e}^{-\beta\mathcal{H}}}{\int \mathrm{d}\Gamma\, \mathrm{e}^{-\beta\mathcal{H}}}$$ com $$\mathrm{d}\Gamma = \prod_{m,\mu} \mathrm{d}\boldsymbol{u}(m,\mu)\, \mathrm{d}\boldsymbol{P}(m,\mu)$$

Mudando para modos normais, temos

$$E = \sum_{\boldsymbol{q},\lambda} \frac{\int \mathrm{d}\Gamma_\lambda(\boldsymbol{q})\, \mathcal{H}_\lambda(\boldsymbol{q}) \mathrm{e}^{-\beta\mathcal{H}_\lambda(\boldsymbol{q})}}{\int \mathrm{d}\Gamma_\lambda(\boldsymbol{q})\, \mathrm{e}^{-\beta\mathcal{H}_\lambda(\boldsymbol{q})}}$$

com

$$\mathrm{d}\Gamma = \prod_{\boldsymbol{q},\lambda} \mathrm{d}|Q_\lambda(\boldsymbol{q})|\, \mathrm{d}|P_\lambda(\boldsymbol{q})|\,.$$

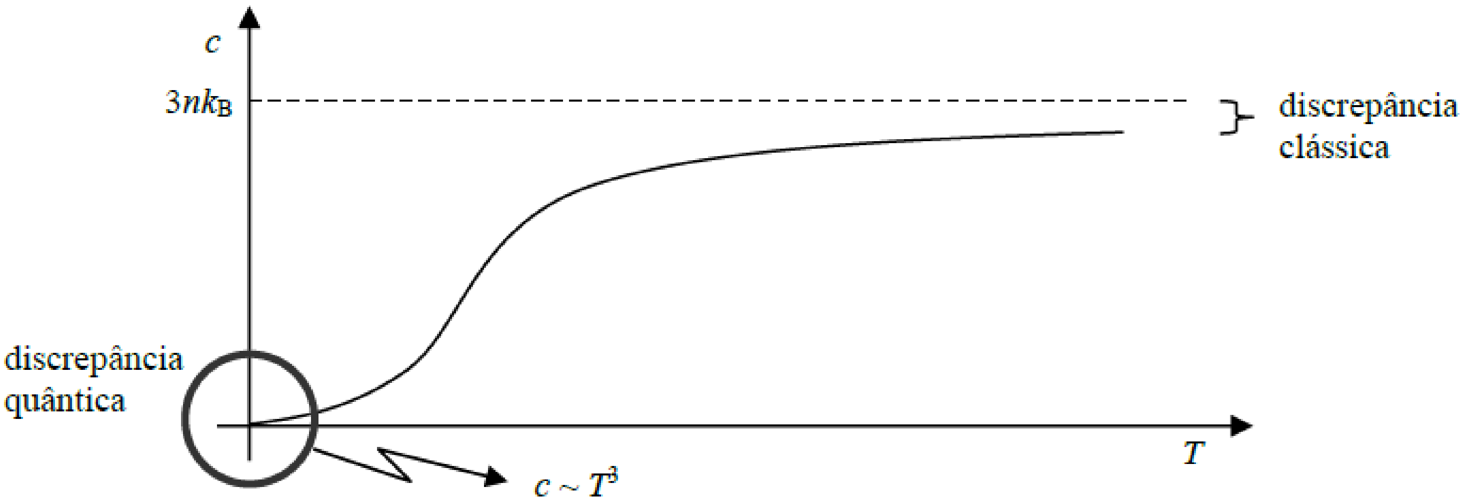
$$\mathcal{H}_\lambda(\boldsymbol{q}) = \tfrac{1}{2}\left\{|P_\lambda(\boldsymbol{q})|^2 + \omega_\lambda^2(\boldsymbol{q})|Q_\lambda(\boldsymbol{q})|^2\right\}$$

$$E = 3Np\, k_\mathrm{B} T\,.$$

$$C_V = \frac{\partial E}{\partial T} = 3Np\, k_\mathrm{B}$$

Lei de Dulong e Petit.

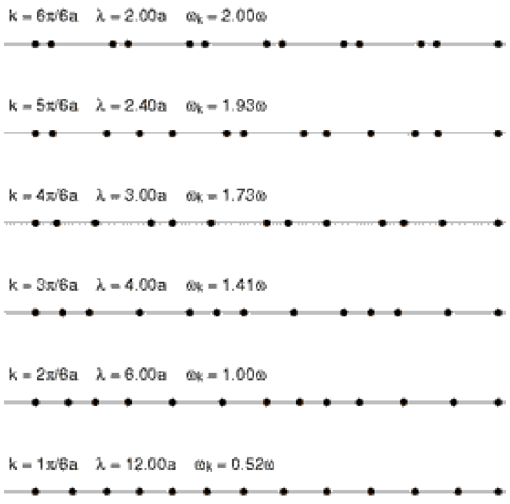
Calor específico



Fônons

- Quantizando o hamiltoniano clássico

$$\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right)$$



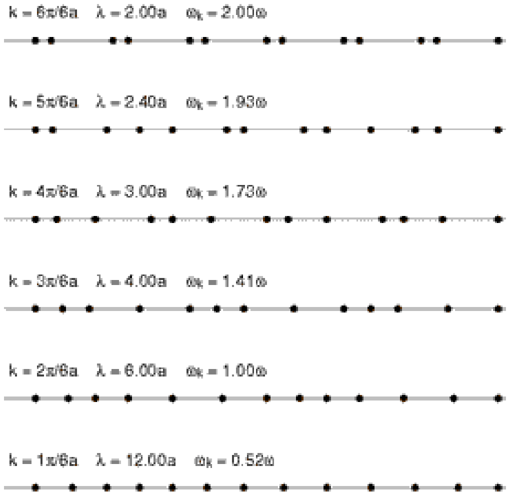
https://en.wikipedia.org/wiki/Phonon

Fônons

- Quantizando o hamiltoniano clássico

$$\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right)$$

$$\boxed{E_n^{(k)} = \hbar\omega_k \left(n + \frac{1}{2} \right)}$$



https://en.wikipedia.org/wiki/Phonon

Probabilidade de encontrarmos um fônon com uma energia En:

$$p(n_{\mathbf{k}s}) = \frac{e^{-\beta E_{n_{\mathbf{k}s}}}}{\sum_{n_{\mathbf{k}s}} e^{-\beta E_{n_{\mathbf{k}s}}}}$$

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Logo, o valor médio de fônons é

$$< n_{\mathbf{k}s} >= \frac{\sum_{n_{\mathbf{k}s}} n_{\mathbf{k}s} e^{-\beta E_{n_{\mathbf{k}s}}}}{\sum_{n_{\mathbf{k}s}} e^{-\beta E_{n_{\mathbf{k}s}}}} = \frac{\sum_{n_{\mathbf{k}s}} n_{\mathbf{k}s} e^{-\beta n_{\mathbf{k}s} \hbar \omega_s(\mathbf{k})}}{\sum_{n_{\mathbf{k}s}} e^{-\beta n_{\mathbf{k}s} \hbar \omega_s(\mathbf{k})}}$$

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$$< n_{\mathbf{k}s} >= -\frac{1}{\beta \hbar} \frac{\partial}{\partial \omega_{\mathbf{k}s}} \ln\left[\sum_{n_{\mathbf{k}s}} e^{-\beta n_{\mathbf{k}s} \hbar \omega_s(\mathbf{k})}\right]$$

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$$u = u_0 + \frac{1}{V} \sum_{\mathbf{k}s} \tfrac{1}{2} \hbar\omega_s(\mathbf{k}) + \frac{1}{V} \sum_{\mathbf{k}s} \frac{\hbar\omega_s(\mathbf{k})}{e^{\beta\hbar\omega_s(\mathbf{k})} - 1}$$

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$$c = \frac{1}{V}\frac{\partial}{\partial T}\sum_{\mathbf{k}s}\frac{\hbar\omega_s(\mathbf{k})}{e^{\beta\hbar\omega_s(\mathbf{k})} - 1}$$

Limite de altas temperaturas:

$$c = \frac{1}{V}\frac{\partial}{\partial T}\sum_{\mathbf{k}s}\frac{\hbar\omega_s(\mathbf{k})}{\beta\hbar\omega_s(\mathbf{k})} = \frac{1}{V}\sum_{\mathbf{k}s} k_B$$

$$= \frac{3N}{V}k_B = 3nk_B$$

OK! Reproduz o limite clássico de Dulong e Petit.

Limite de altas temperaturas:

$$c = \frac{1}{V}\frac{\partial}{\partial T}\sum_{\boldsymbol{k}s}\frac{\hbar\omega_s(\boldsymbol{k})}{\beta\hbar\omega_s(\boldsymbol{k})} = \frac{1}{V}\sum_{\boldsymbol{k}s} k_B$$

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Limite de baixas temperaturas: Modelo de Einstein

$$\omega_s(\mathbf{k}) = \omega_E$$

→ Fônons puramente óticos

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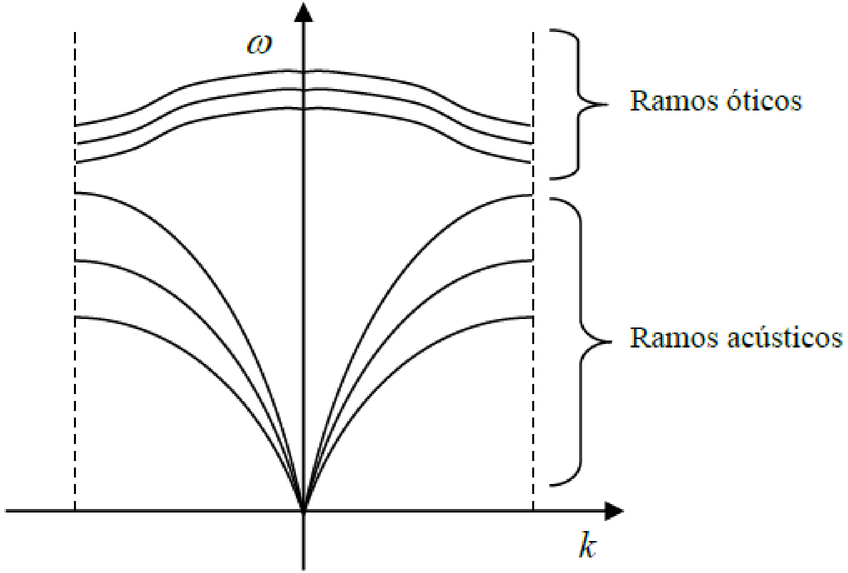

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$$c = \frac{1}{V}\frac{\partial}{\partial T}\sum_{\mathbf{k}s}\frac{\hbar\omega_E}{e^{\beta\hbar\omega_E}-1} = 3n\frac{\partial}{\partial T}\left[\frac{\hbar\omega_E}{e^{\hbar\omega_E/k_BT}-1}\right]$$

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$$= \frac{3n\hbar\omega_E e^{\hbar\omega_E/k_BT}\left(\hbar\omega_E/k_BT^2\right)}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2}$$

$$= 3nk_B\frac{e^{\hbar\omega_E/k_BT}\left(\hbar\omega_E/k_BT\right)^2}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2}$$

$$c \approx e^{-\hbar\omega_E/k_BT}$$

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$$c = \frac{1}{V}\frac{\partial}{\partial T}\sum_{\boldsymbol{k}s}\frac{\hbar\omega_s(\boldsymbol{k})}{\beta\hbar\omega_s(\boldsymbol{k})} = \frac{1}{V}\sum_{\boldsymbol{k}s} k_B$$

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Limite de baixas temperaturas: Modelo de Einstein

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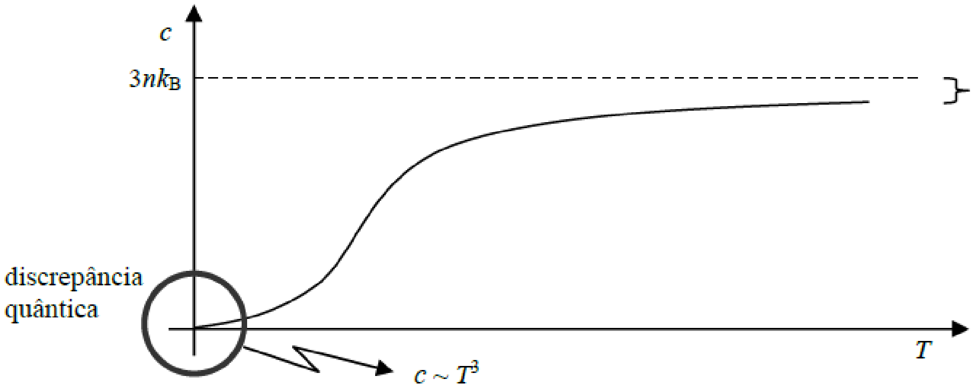

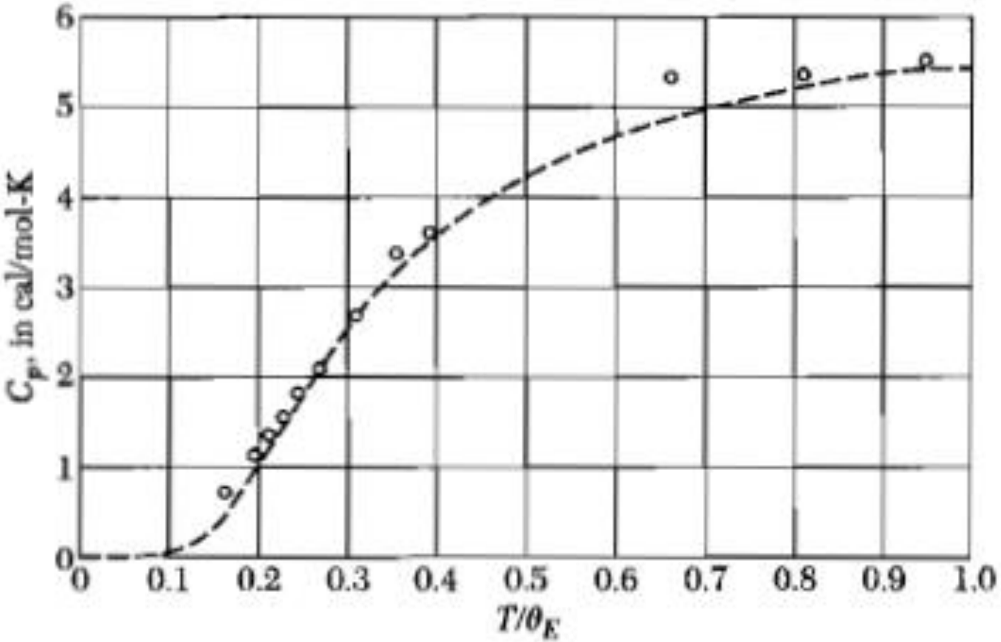

Figure 11 Comparison of experimental values of the heat capacity of diamond with values calculated on the earliest quantum (Einstein) model, using the characteristic temperature $\theta_E = \hbar\omega/k_B = 1320$ K. To convert to J/mol-deg, multiply by 4.186.

Limite de baixas temperaturas: Modelo de Debye

$$\omega_s(\mathbf{k}) = ck$$

Limite de baixas temperaturas: Modelo de Debye

$$\omega_s(\mathbf{k}) = ck$$

$$c = \frac{1}{V}\frac{\partial}{\partial T}\sum_{\mathbf{k}s}\frac{\hbar ck}{e^{\beta\hbar ck}-1} = \frac{3}{V}\frac{\partial}{\partial T}\frac{V}{(2\pi)^3}\int_0^{k_D} 4\pi k^2 \frac{\hbar ck}{e^{\beta\hbar ck}-1}dk$$

$$\frac{4}{3}\pi k_D^3 = N_{cel}\frac{(2\pi)^3}{V} \Rightarrow k_D = \left(\frac{6N_{cel}\pi^2}{V}\right)^{1/3}$$

Limite de baixas temperaturas: Modelo de Debye

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$$c = \frac{1}{V}\frac{\partial}{\partial T}\frac{V}{(2\pi)^3}4\pi\int_0^{k_D}\frac{\hbar ck^3}{e^{\beta\hbar ck}-1}dk = \frac{1}{2\pi^2}\frac{\hbar c\,\partial}{\partial T}\int_0^{k_D}\frac{k^3}{e^{\beta\hbar ck}-1}dk$$

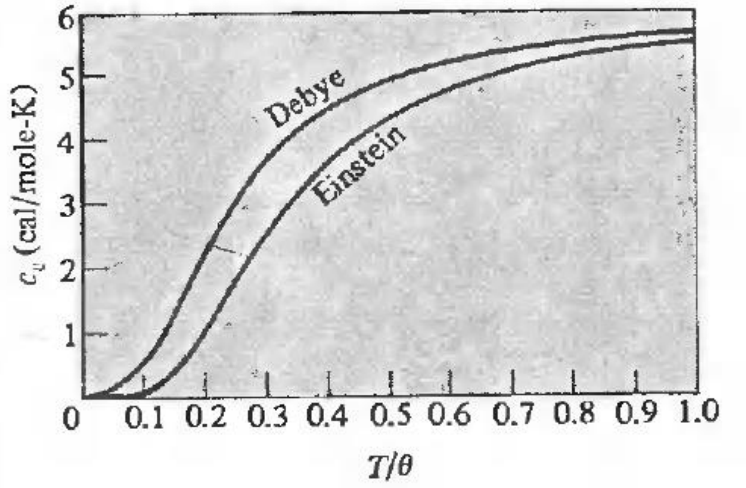
$$= \frac{1}{2\pi^2}\frac{\hbar c}{}\int_0^{k_D}\frac{k^3 e^{\beta\hbar ck}}{(e^{\beta\hbar ck}-1)^2}\frac{\hbar ck}{k_B T^2}dk$$

$$x = \frac{\hbar ck}{k_B T} \qquad \Theta_D = \frac{\hbar ck_D}{k_B}$$

$$c = \frac{1}{2\pi^2}\frac{\hbar c}{}\int_0^{\Theta_D/T}\frac{k_B}{\hbar c}\left(\frac{k_B T}{\hbar c}\right)^3\frac{x^4 e^x}{(e^x-1)^2}dx$$

$$c = 9nk_B\left(\frac{T}{\Theta_D}\right)^3\int_0^\infty \frac{x^4e^x}{(e^x-1)^2}dx$$

$$c = \frac{12\pi^4}{5}nk_B\left(\frac{T}{\Theta_D}\right)^3$$



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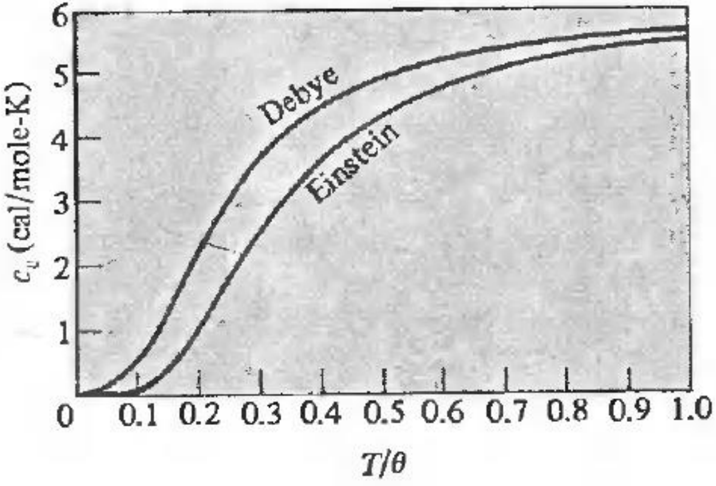


Table 23.2
TEMPERATURE DEPENDENCE OF THE DEBYE SPECIFIC HEAT[a]

T/Θ_D	$c_v/3nk_B$	T/Θ_D	$c_v/3nk_B$	T/Θ_D	$c_v/3nk_B$
0.00	0	0.35	0.687	0.70	0.905
0.05	0.00974	0.40	0.746	0.75	0.917
0.10	0.0758	0.45	0.791	0.80	0.926
0.15	0.213	0.50	0.825	0.85	0.934
0.20	0.369	0.55	0.852	0.90	0.941
0.25	0.503	0.60	0.874	0.95	0.947
0.30	0.608	0.65	0.891	1.00	0.952

[a] The table entries are the ratios of the Debye to the Dulong-Petit specific heats, that is, $c_v/3nk_B$, with c_v given by (23.26).
Source: J. de Launay, *Solid State Physics*, vol. 2, F. Seitz and D. Turnbull, eds., Academic Press, New York, 1956.

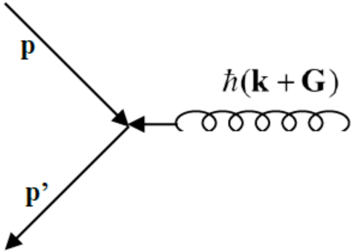
Table 23.3

DEBYE TEMPERATURES FOR SELECTED ELEMENTS[a]

ELEMENT	Θ_D (K)	ELEMENT	Θ_D (K)
Li	400	A	85
Na	150	Ne	63
K	100		
		Cu	315
Be	1000	Ag	215
Mg	318	Au	170
Ca	230		
		Zn	234
B	1250	Cd	120
Al	394	Hg	100
Ga	240		
In	129	Cr	460
Tl	96	Mo	380
		W	310
C (diamond)	1860	Mn	400
Si	625	Fe	420
Ge	360	Co	385
Sn (grey)	260	Ni	375
Sn (white)	170	Pd	275
Pb	88	Pt	230
As	285	La	132
Sb	200	Gd	152
Bi	120	Pr	74

[a] The temperatures were determined by fitting the observed specific heats c_v to the Debye formula (23.26) at the point where $c_v = 3nk_B/2$. Source: J. de Launay, *Solid State Physics*, vol. 2, F. Seitz and D. Turnbull, eds., Academic Press, New York, 1956.

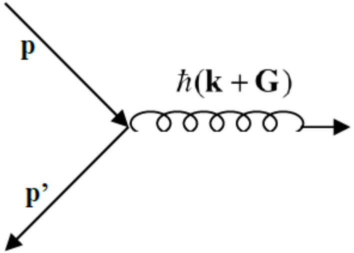
Momento Cristalino



$$\boldsymbol{u}_{\boldsymbol{k}}(\boldsymbol{R},t) = \frac{1}{\sqrt{M}}\hat{\boldsymbol{\varepsilon}}(\boldsymbol{k})e^{i(\boldsymbol{k}\cdot\boldsymbol{R}-\omega t)}$$

$$\boldsymbol{P}_{tot} = M\frac{d}{dt}\sum_{\boldsymbol{R}}\boldsymbol{u}_{\boldsymbol{k}}(\boldsymbol{R},t) = -i\omega\sqrt{M}e^{-i\omega t}\hat{\boldsymbol{\varepsilon}}\sum_{\boldsymbol{R}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$= \begin{cases} 0, \text{ se } \mathbf{k} \neq 0 \\ N, \text{ se } \mathbf{k} = 0 \end{cases}$$



$$\mathbf{p}' - \mathbf{p} = \mp\hbar(\mathbf{k} + \mathbf{G})$$
$$E' - E = \mp\hbar\omega_s(\mathbf{k})$$

$$\hbar(\mathbf{q}' - \mathbf{q}) = \mp\hbar\mathbf{G} \Rightarrow \Delta\mathbf{q} = \mathbf{G}$$

Espalhamento elástico satisfaz a condição de von Laue

Acoplamento Elétron-íon

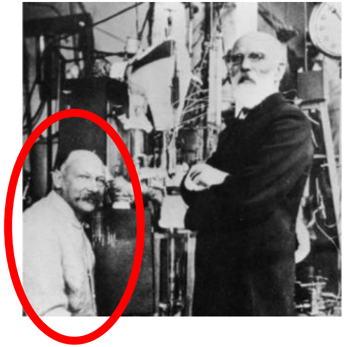
$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 - \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

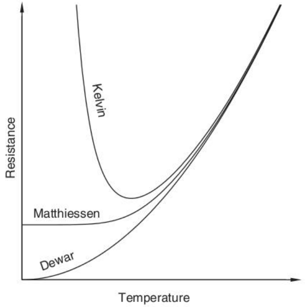
$$-\sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|},$$

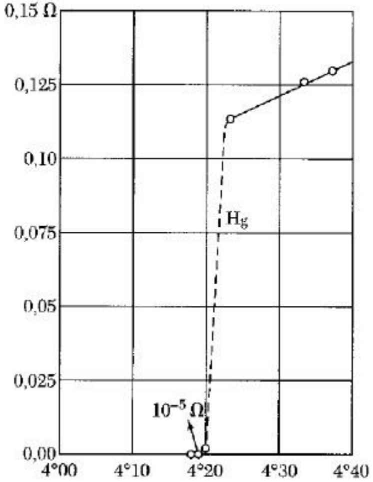
Conventional Superconductivity

Electron-phonon Interaction

Heike Kamerlingh Onnes

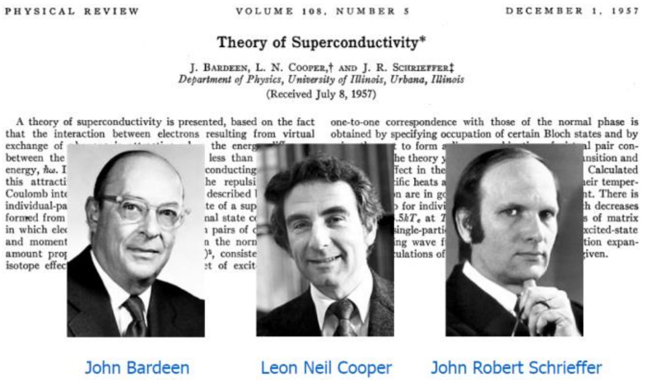






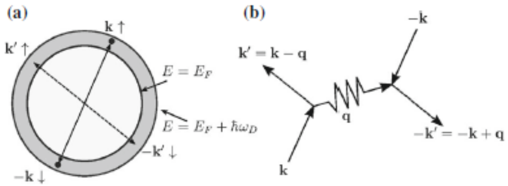
$$T_c \propto M^{-\alpha}$$

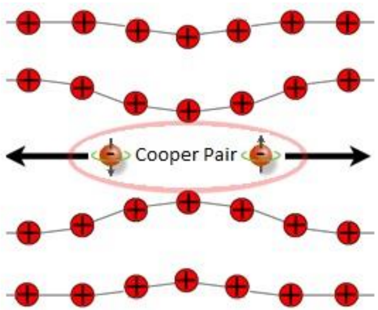
Vibrações da rede cristalina (fônons)


PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Theory of Superconductivity*

J. Bardeen,† L. N. Cooper,† and J. R. Schrieffer‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)





$$V^0_{\text{eff}}(\mathbf{q},\omega) = W(q)\,\frac{\omega^2}{\omega^2 - \Omega^2 + i\tilde{\eta}}.$$

Introduction

Peierls Instability → The standard explanation for charge-density wave (CDW) formation

"Recipe" for CDW …

- One-dimensional system;
- Fermi Surface Nesting (FSN);
- Create an electronic instability (or a lattice distortion)

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- Fermi Surface Nesting (FSN);
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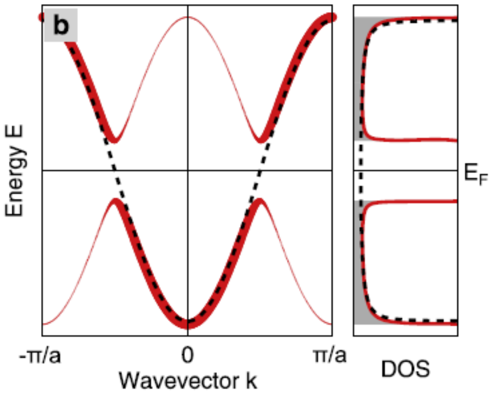
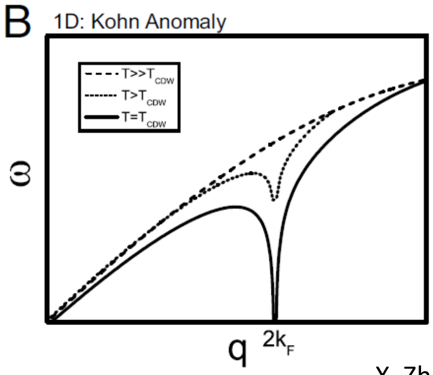
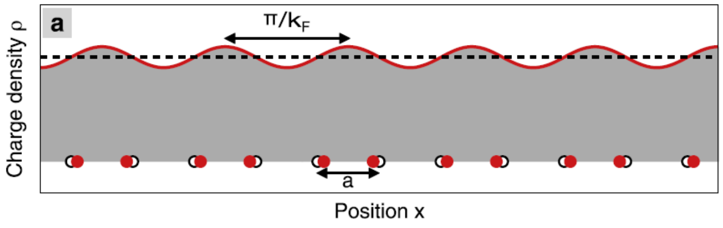
→

- Charge gap at Fermi level (metal-insulator transition);
- Phonon softening at **q**=2**k**$_F$;
- Permanent lattice distortion.



K. Rossnagel, J. Phys.: Condens. Matter **23** 213001 (2011)





X. Zhu et al., *Proc. Natl Acad. Sci. USA* **112**, 2367–2371 (2015)

Introduction

Peierls Instability

Linear Response Theory

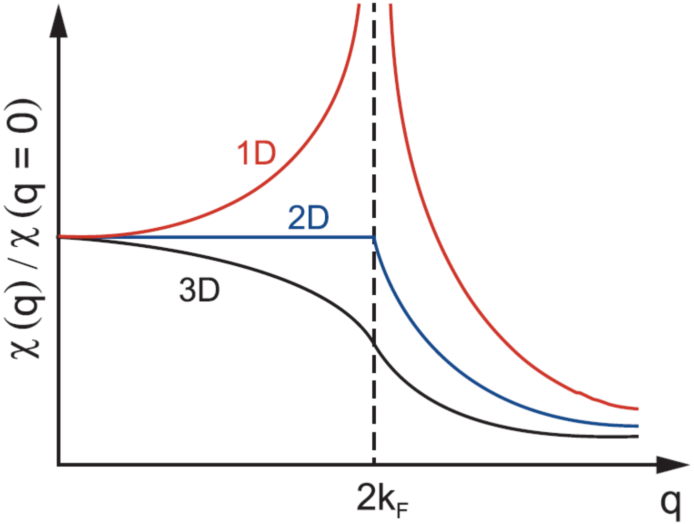
$$\rho^{\mathrm{ind}}(\vec{r},\omega) = e^2 \int d\vec{r}' \chi(\vec{r},\vec{r}',\omega)\Phi^{\mathrm{tot}}(\vec{r}',\omega)$$

Fermi gas

$$\begin{cases} \chi'(\mathbf{q}) = \sum_{\mathbf{k}} \dfrac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k+q}})}{\varepsilon_k - \varepsilon_{\mathbf{k+q}}}, \\ \lim_{\omega\to 0} \chi''(\mathbf{q},\omega)/\omega = \sum_k \delta(\varepsilon_k - \varepsilon_F)\,\delta(\varepsilon_{k+q} - \varepsilon_F) \end{cases}$$

Electronic susceptibility

C.-W. Chen et al., Rep. Prog. Phys. **79** 084505 (2016)



One-dimensional systems are highly susceptible at $\mathbf{q}=2\mathbf{k}_F$

1D: $\mathrm{Re}\chi_0 \propto -\dfrac{1}{2q} \ln\left|\dfrac{1+q/2}{1-q/2}\right|$

2D: $\mathrm{Re}\chi_0 \propto \begin{cases} -(1 - \sqrt{1-(2/q)^2}), q \ge 2k_F \\ -1/E_F, q < 2k_F \end{cases}$

3D: $\mathrm{Re}\chi_0 \propto -\left[1 + \dfrac{1-(q/2)^2}{q} \ln\left|\dfrac{1+q/2}{1-q/2}\right|\right]$

Introduction

Peierls Instability

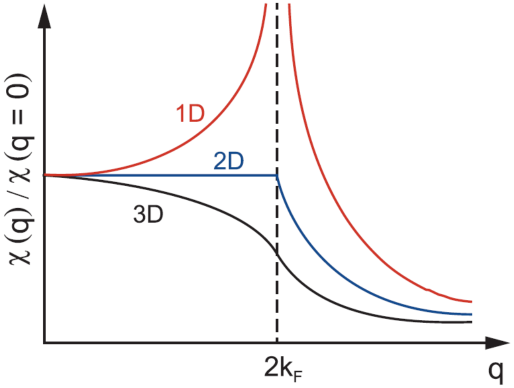
$$\phi^{\text{ind}}(\mathbf{q}) = g\rho^{\text{ind}}(\mathbf{q})$$

$$\rho^{\text{ind}}(\mathbf{q}) = \chi_0(\mathbf{q})\phi(\mathbf{q}) = \chi_0(\mathbf{q})\left[\phi^{\text{ext}}(\mathbf{q}) + \phi^{\text{ind}}(\mathbf{q})\right]$$

$$\rho^{\text{ind}}(\mathbf{q},T) = \frac{\chi_0(\mathbf{q},T)\phi^{\text{ext}}(\mathbf{q})}{1 - g\chi_0(\mathbf{q},T)} \qquad 1 - g\chi_0(\mathbf{q},T) = 0$$

Fröhlich Hamiltonian

$$H_{\text{PI}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a^+_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^+_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} g_{\mathbf{q}} a^+_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}} (b^+_{-\mathbf{q}} + b_{\mathbf{q}}),$$



C.-W. Chen et al., Rep. Prog. Phys. **79** 084505 (2016)

For ideal 1D systems *any* Electron-Phonon Coupling leads to CDW!

Criterion to CDW (Perturbation theory)

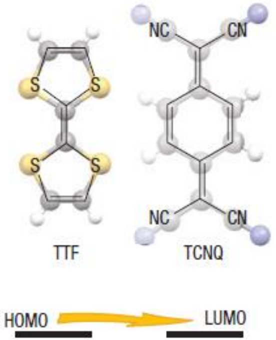
$$\frac{4g^2_{\mathbf{q}}}{\hbar\omega_{\mathbf{q}}} > \frac{1}{\chi_0(\mathbf{q})}$$

More generally

$$\frac{4g^2_{\mathbf{q}}}{\hbar\omega_{\mathbf{q}}} - 2U_{\mathbf{q}} + V_{\mathbf{q}} \geqslant \frac{1}{\chi_0(\mathbf{q})}$$

Organic molecular crystal
tetrathiafulvalene-tetracyanoquinodimethane
(TTF-TCNQ)

Introduction



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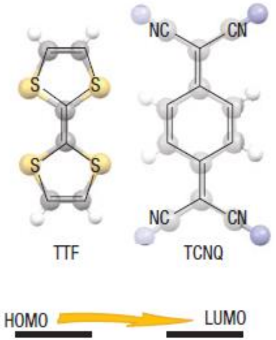


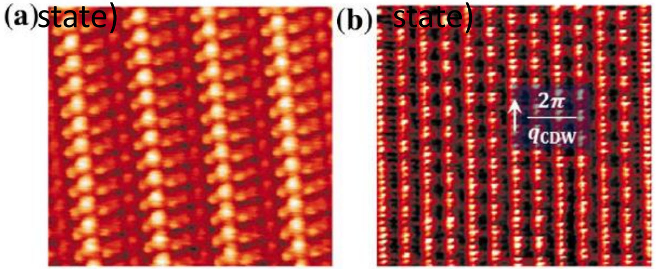
Introduction

X. Zhu, et al. *Advances in Physics: X,* 2(3), 622-640 (2017).

STM measurements

63 K (normal state)

36 K (CDW state)

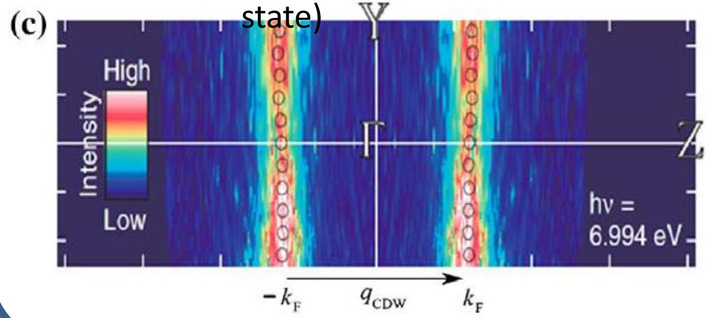


TCNQ

TTF

ARPES measurements

60 K (normal state)



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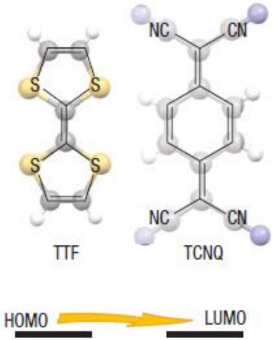
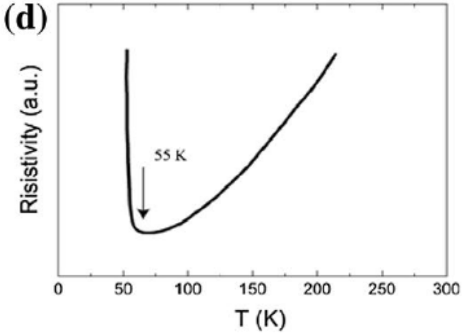
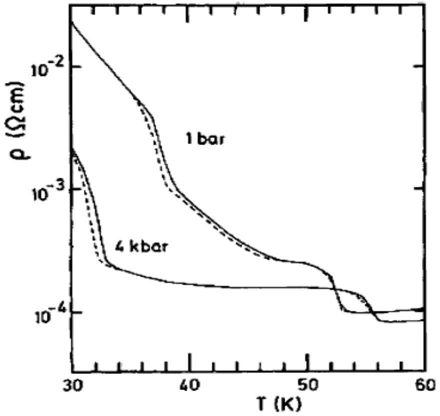


Resistivity





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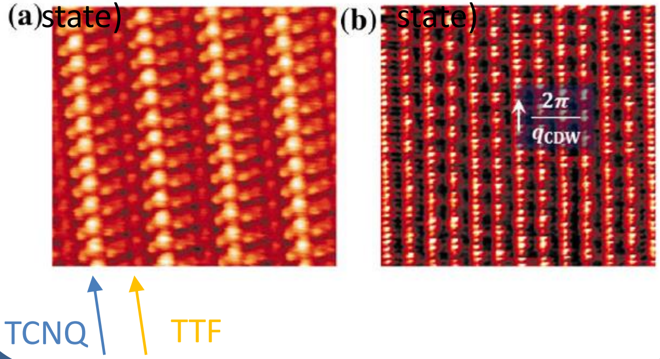
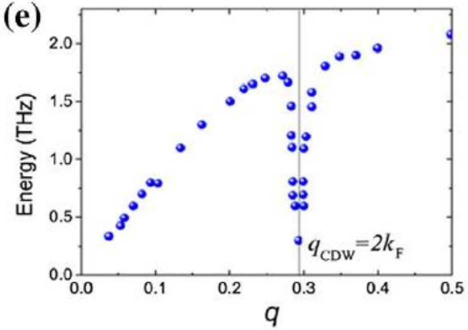


Inelastic neutron scattering



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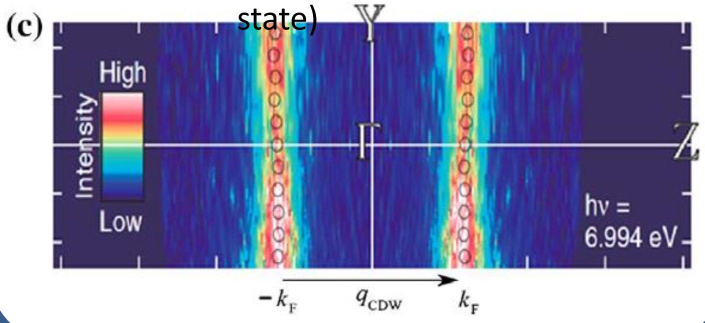

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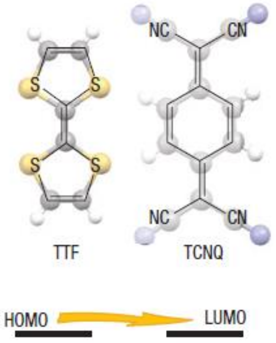

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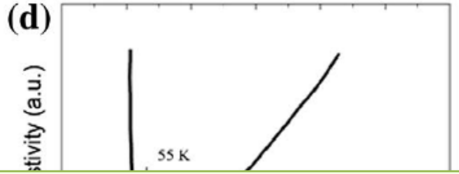

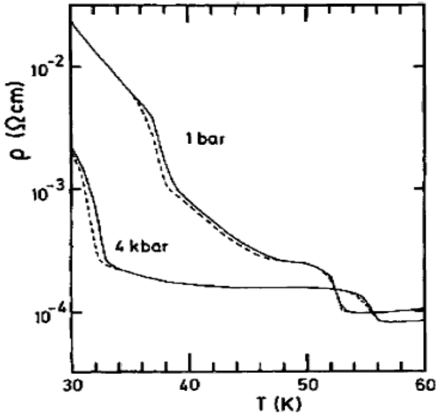

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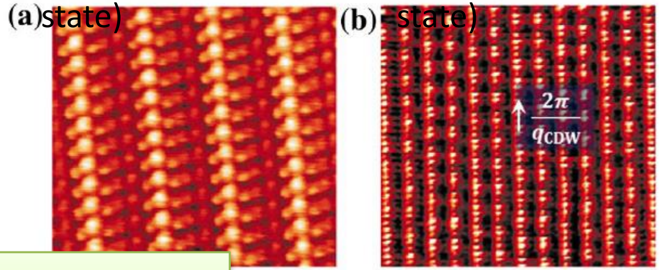
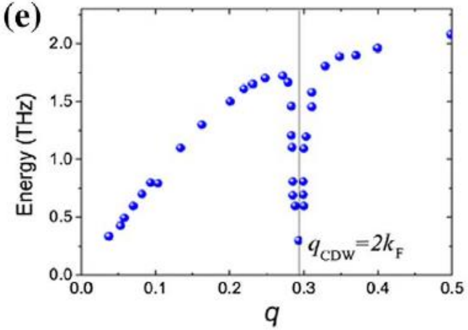


✓ Peierls' argument

Inelastic neutron scattering



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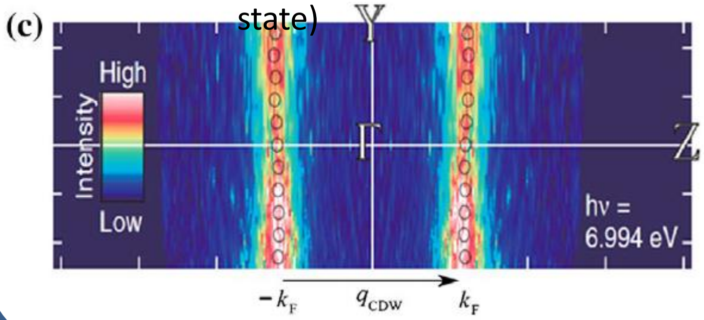
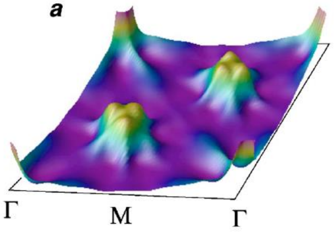


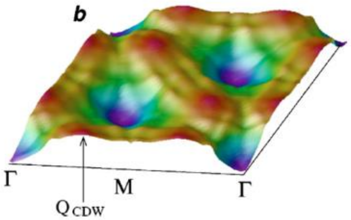
Introduction

The Nature of CDW

NbSe2 → Quasi-2D material



$$\lim_{\omega\to 0} \chi''(\mathbf{q},\omega)/\omega$$



$$\chi'(\mathbf{q})$$

M. D. Johannes, I. I. Mazin, and C. A. Howells, Phys. Rev. B **73**, 205102 (2006).

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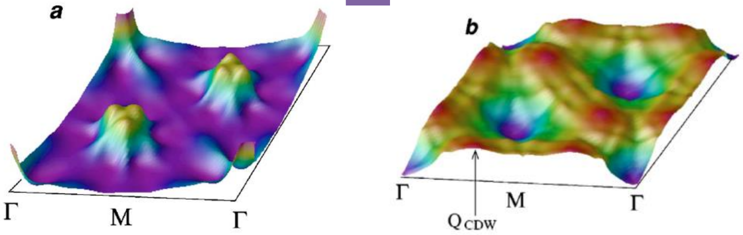

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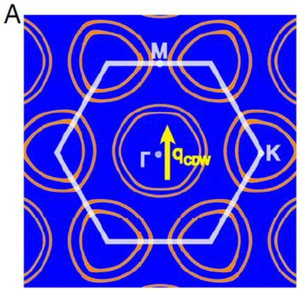

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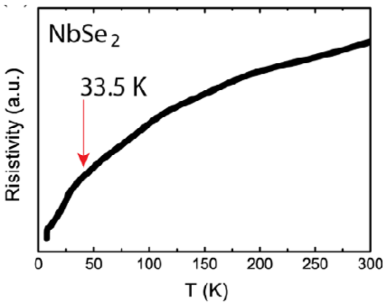
- No electronic divergence
- No FSN
- No metal-insulator transition

CDW at

$q_{CDW} = (2/3)|\Gamma M|$



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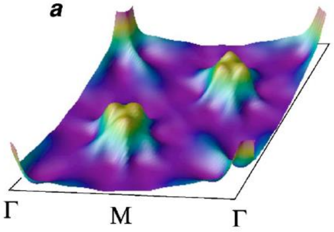

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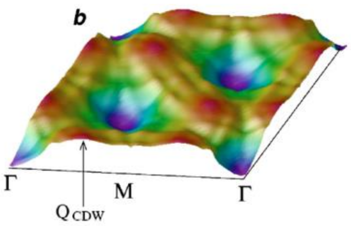

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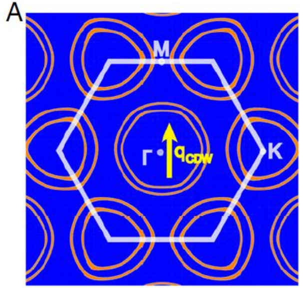

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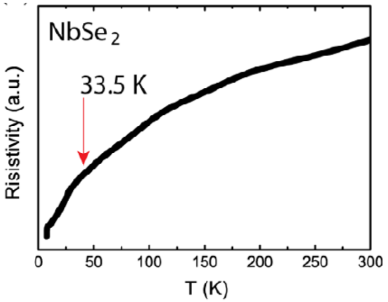

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✘ ~~Peierls' argument~~

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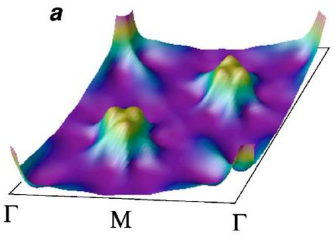

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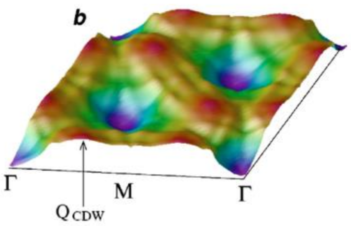

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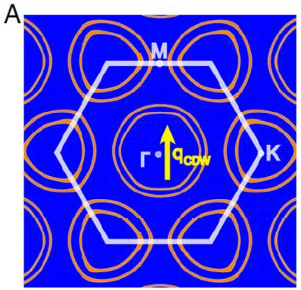

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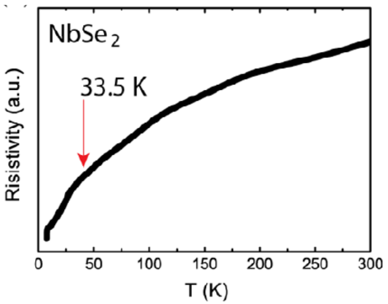

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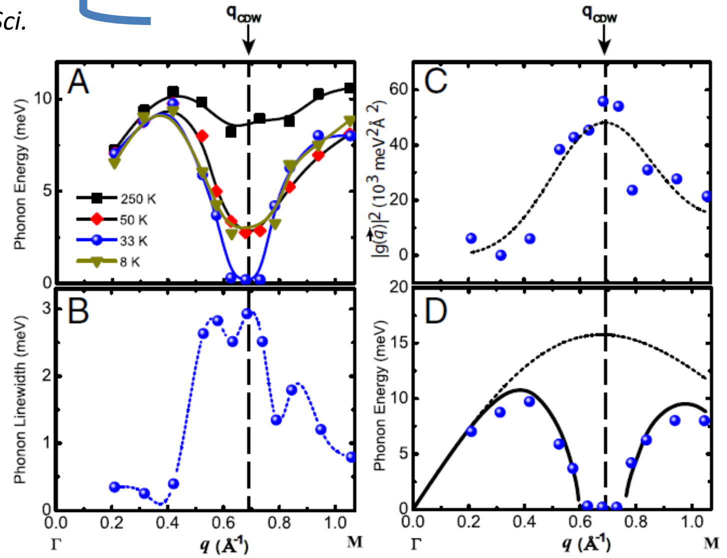
$$\Gamma_{EPC}(\vec{q}) = -2|g(\vec{q})|^2 \ \mathrm{Im}[\chi(\omega,\vec{q})]$$

Measurements of phonon linewidth provide a direct measurement of EPC.

Strong Evidence of a (non-Peierls) CDW by EPC



Introduction

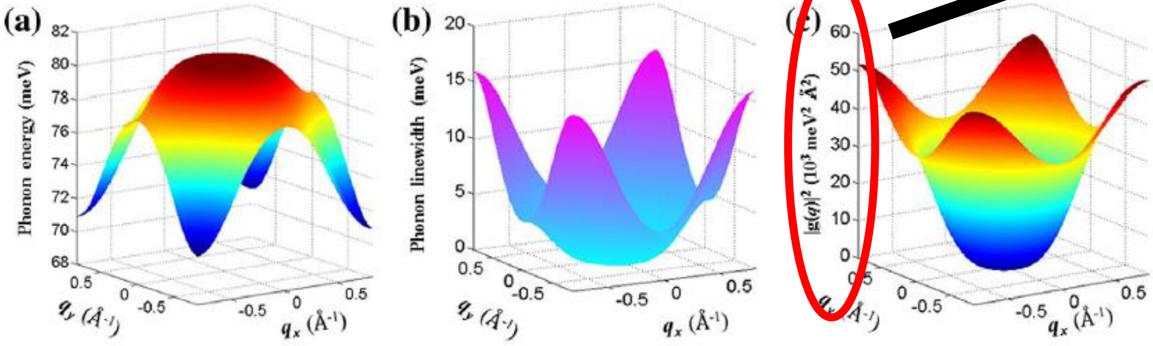
The Nature of CDW

Cuprates

On the other hand …

optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$

(ARPES measurements)



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Strong EPC

But…

No evidence of CDW!

Electron-electron interactions ?