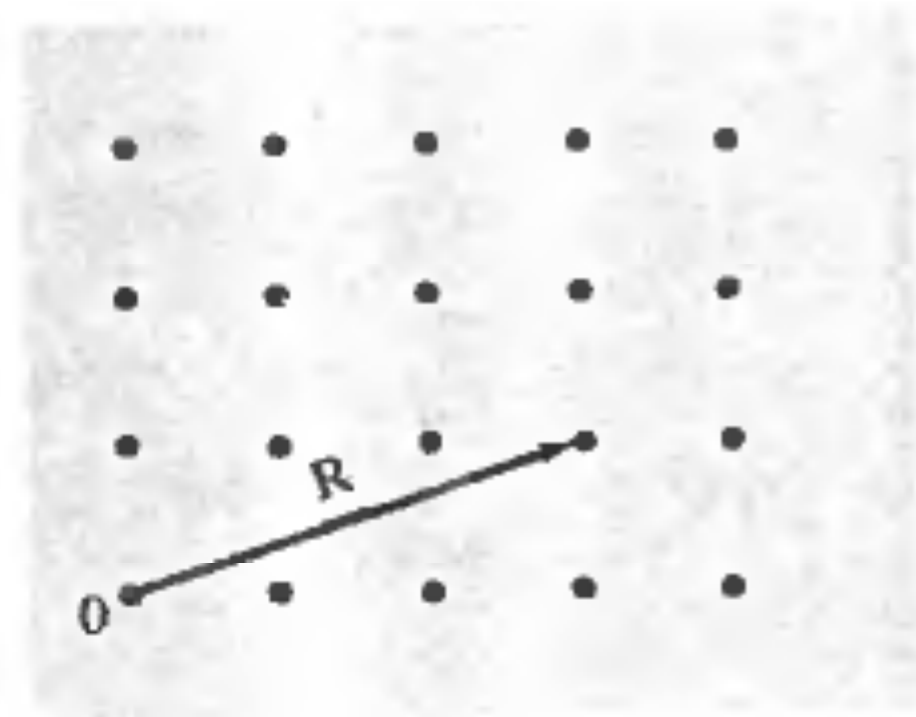
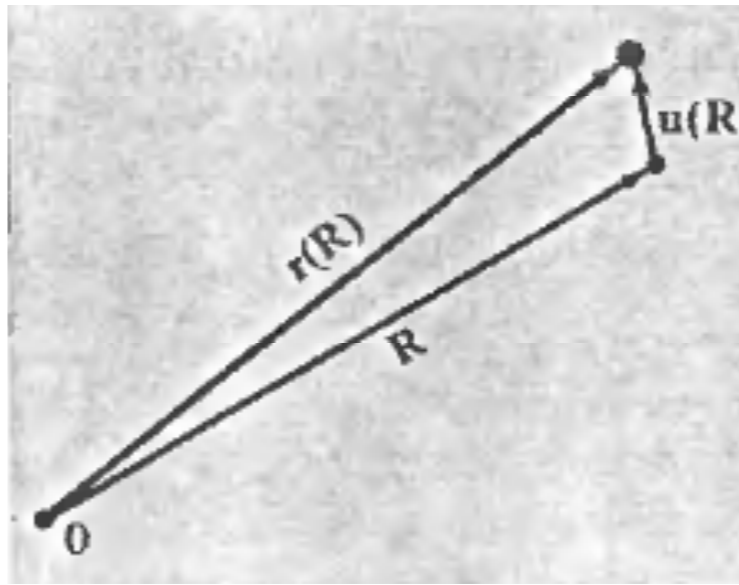


fononi
22 dicembre 2021

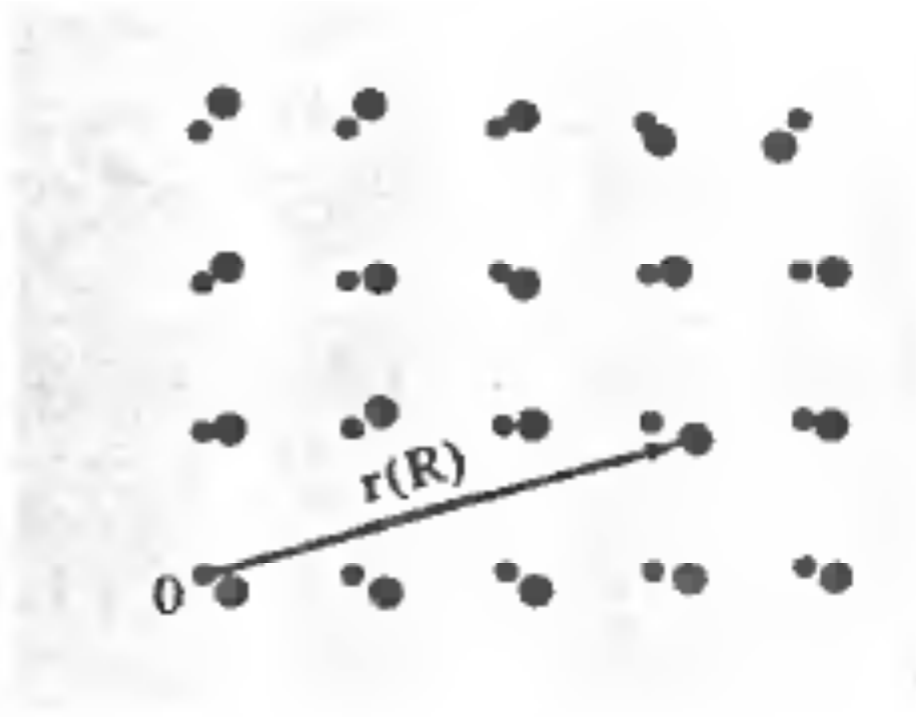
M. Peressi

- rilasciamo l'ipotesi di ioni rigidamente bloccati nei **siti $\{R\}$ dei reticoli di Bravais** (e eventualmente posizioni di base)
- queste posizioni vanno considerate di **equilibrio**
- con **spostamenti $u(R)$ "piccoli"** rispetto alle distanze interatomiche

$$\mathbf{r}(\mathbf{R}) = \mathbf{R} + \mathbf{u}(\mathbf{R})$$



(a)

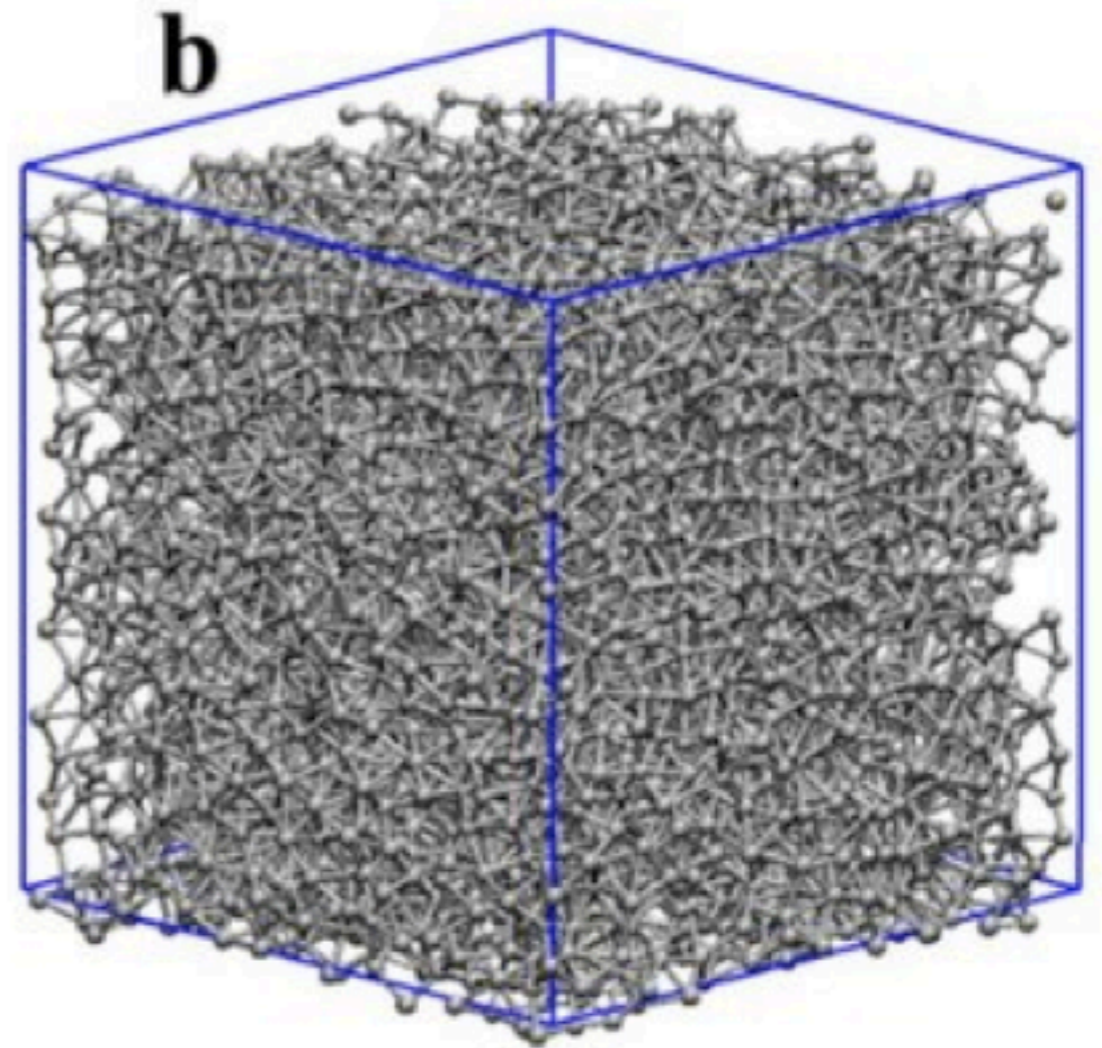
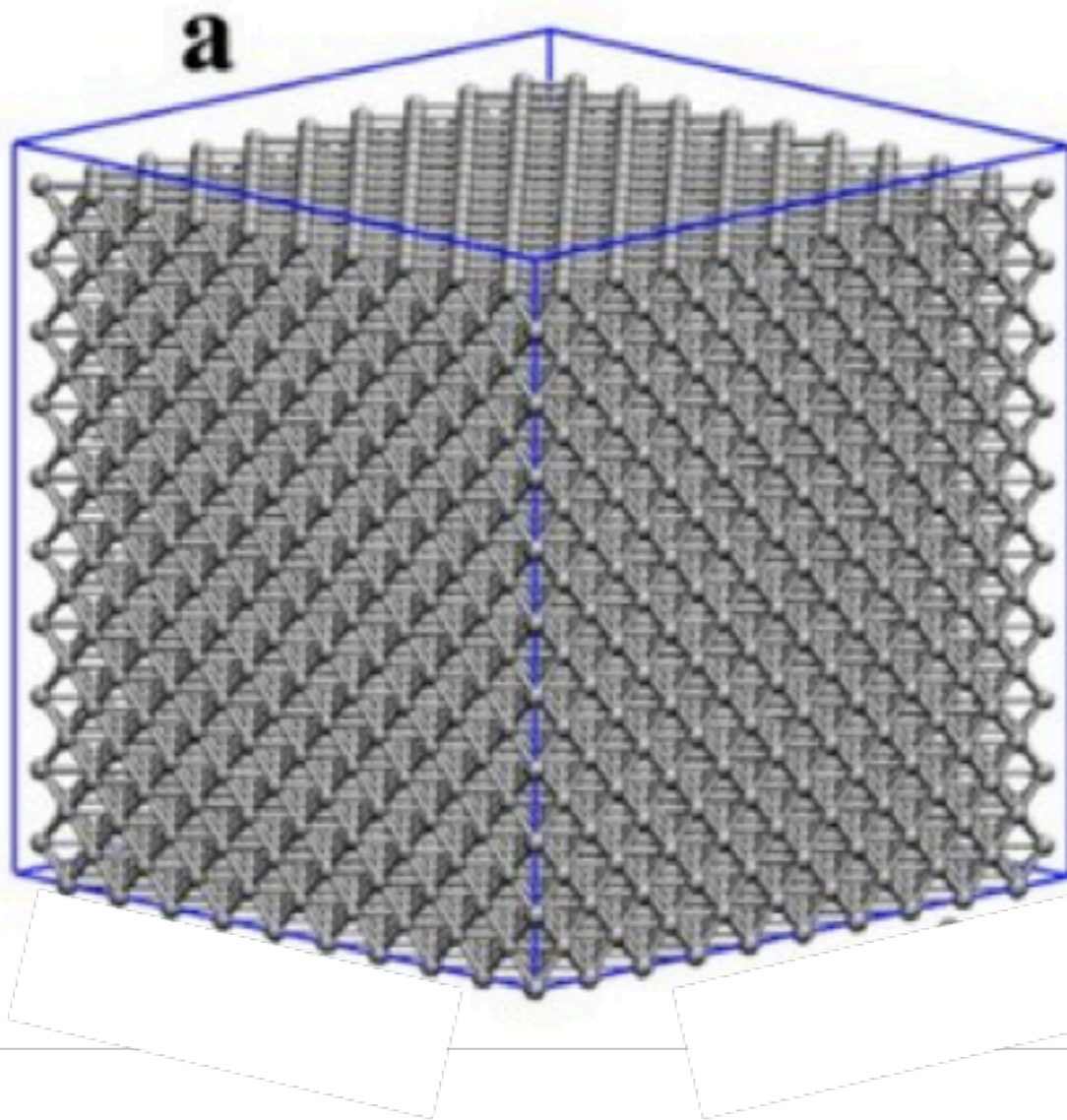


(b)

Figure 22.1

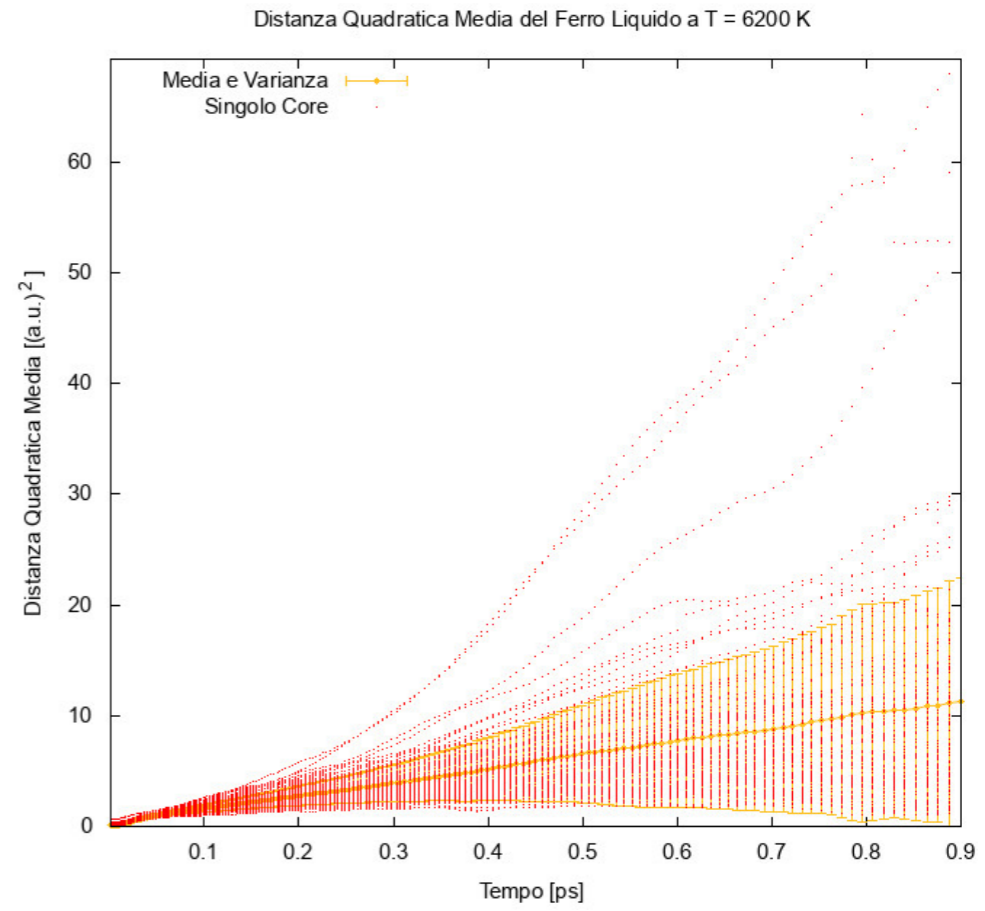
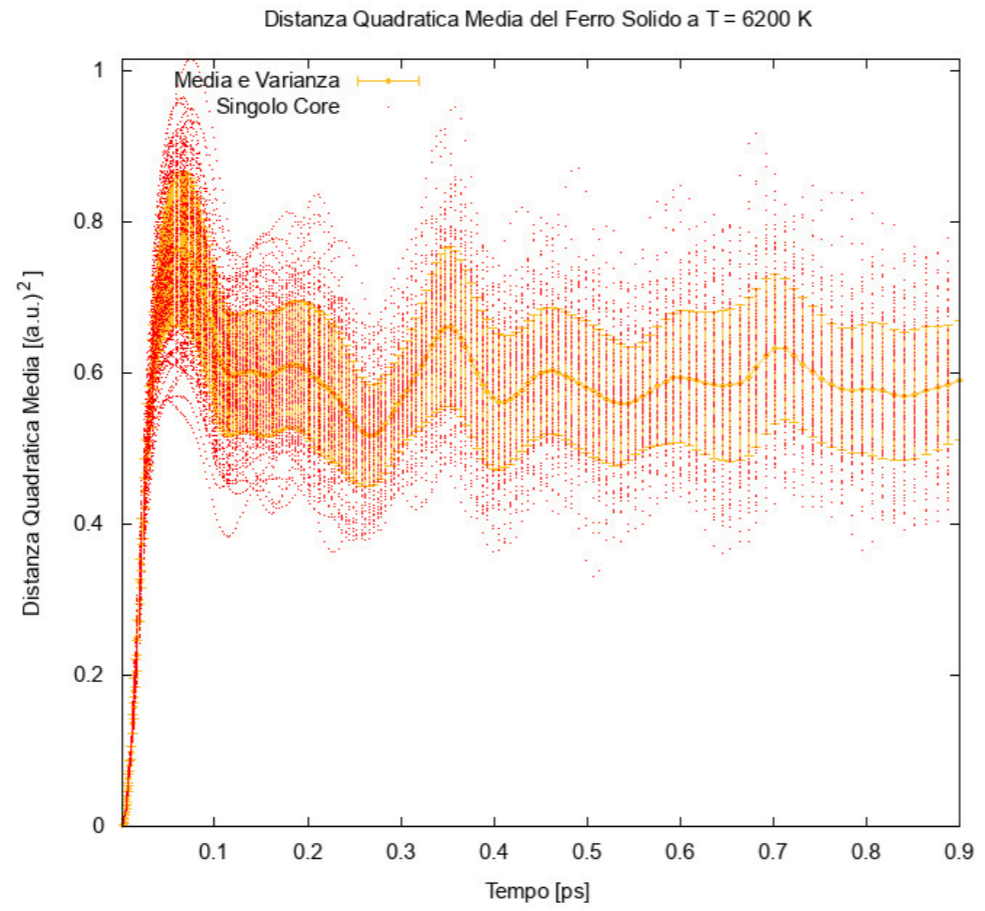
(a) The Bravais lattice of points, specified by vectors \mathbf{R} . (b) A particular instantaneous configuration of ions. The ion whose mean position is \mathbf{R} is found at $\mathbf{r}(\mathbf{R})$.

ovviamente una configurazione di un solido cristallino con spostamenti “piccoli” degli ioni è ben diversa da una configurazione di liquido

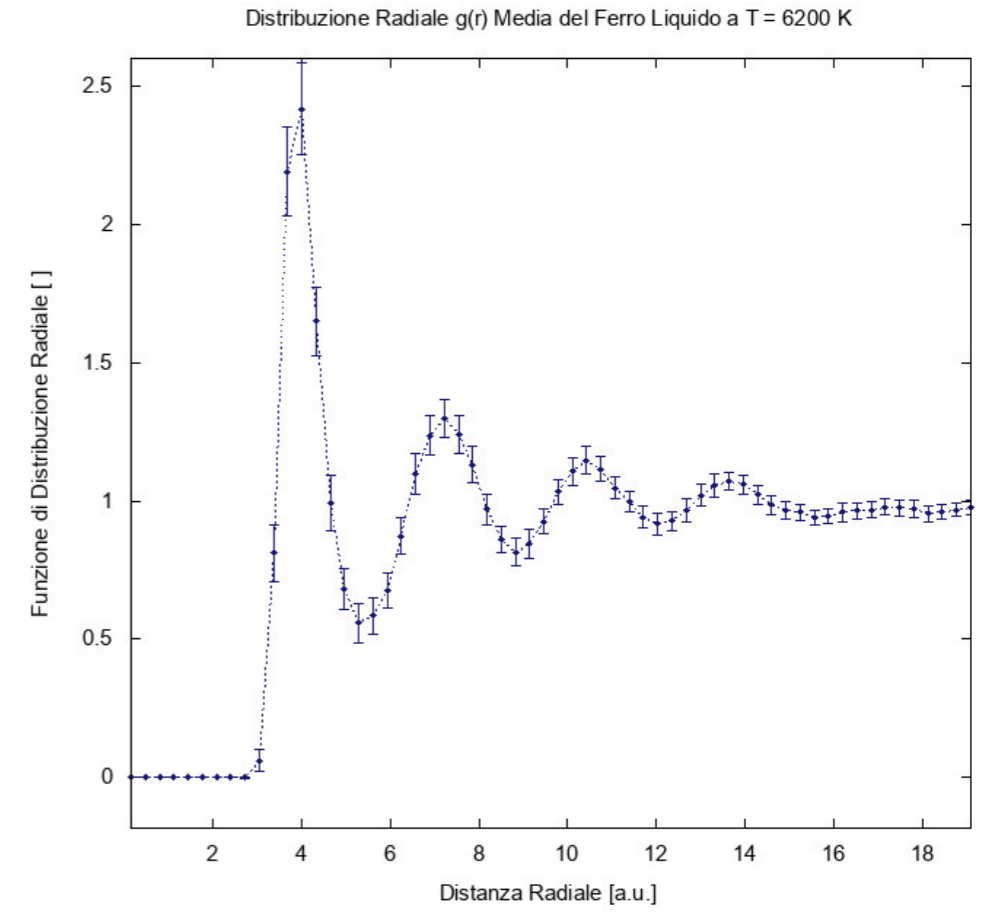
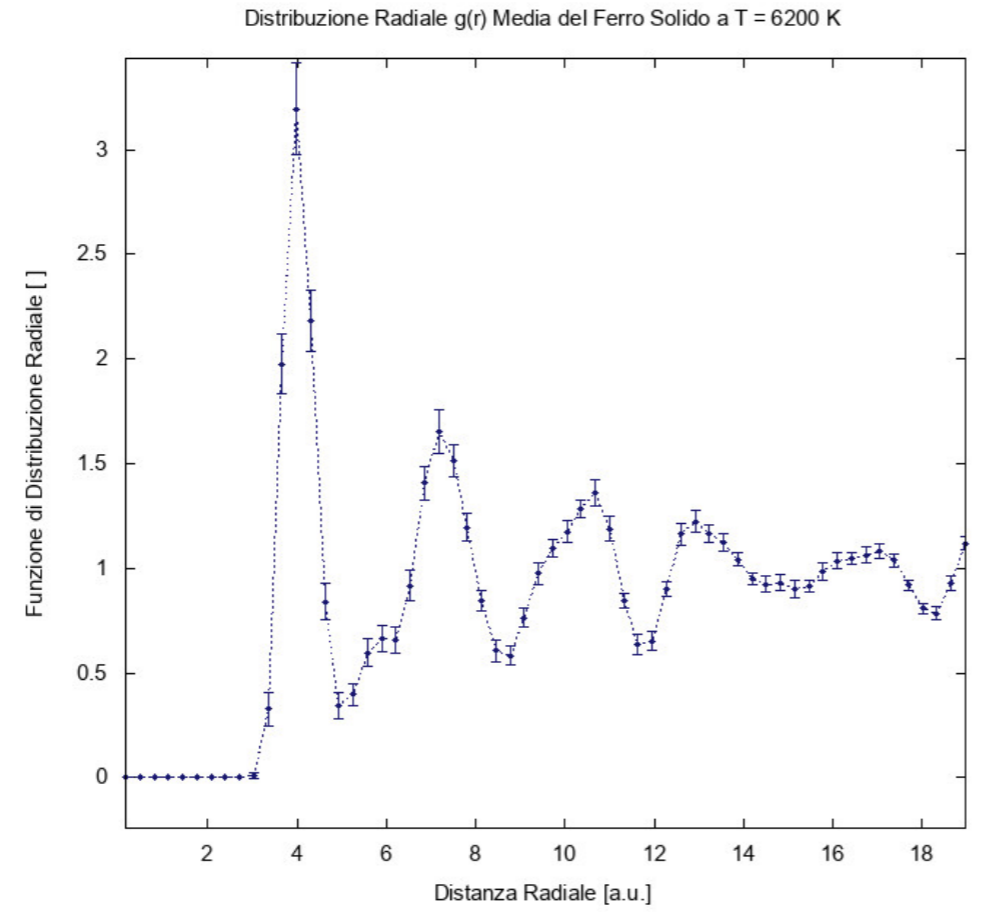


La differenza tra solido cristallino e liquido si vede bene quantitativamente attraverso queste quantità (tesi LMW. Zuccolin, Dic. 2022):

Mean square distance



Radial distribution function



(a) Solido.

(b) Liquido.

static lattice model

total potential energy of the crystal

as sum of 2-body terms (Φ effective potential !)

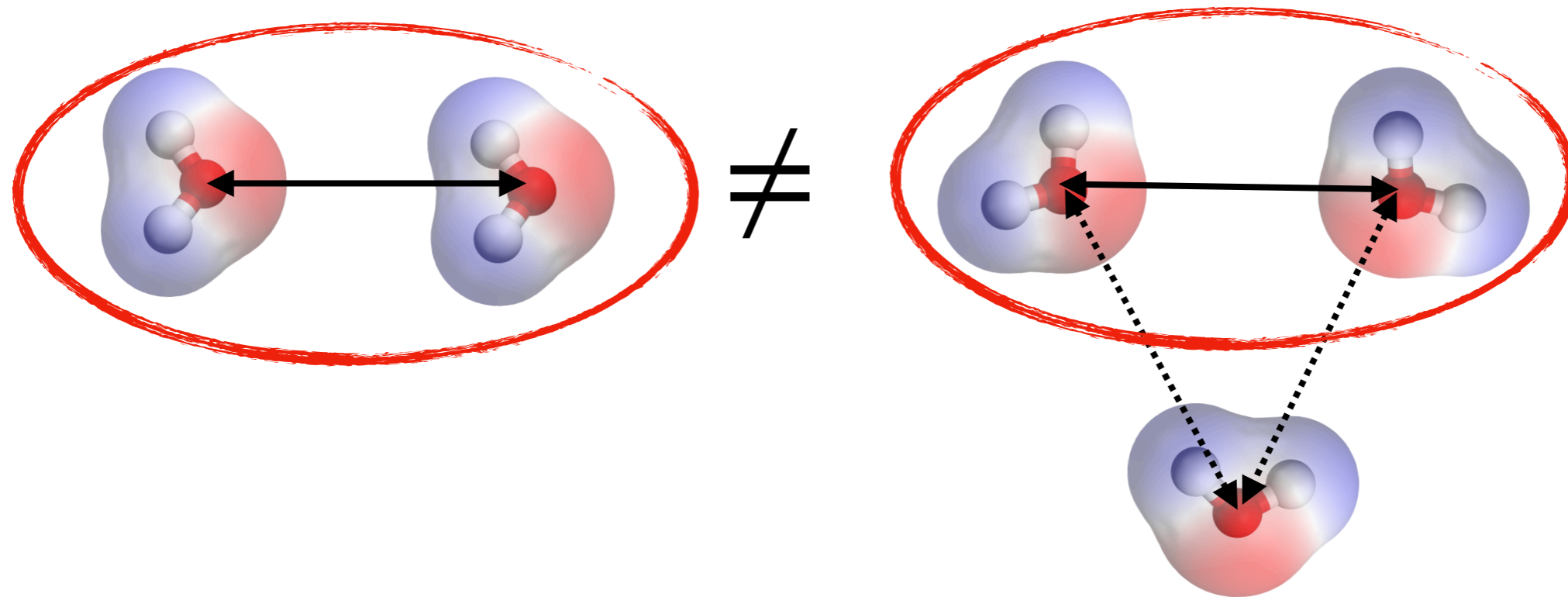
$$U = \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \phi(\mathbf{R} - \mathbf{R}') = \frac{N}{2} \sum_{\mathbf{R} \neq \mathbf{0}} \phi(\mathbf{R})$$

(no self-interaction)

Including displacements:

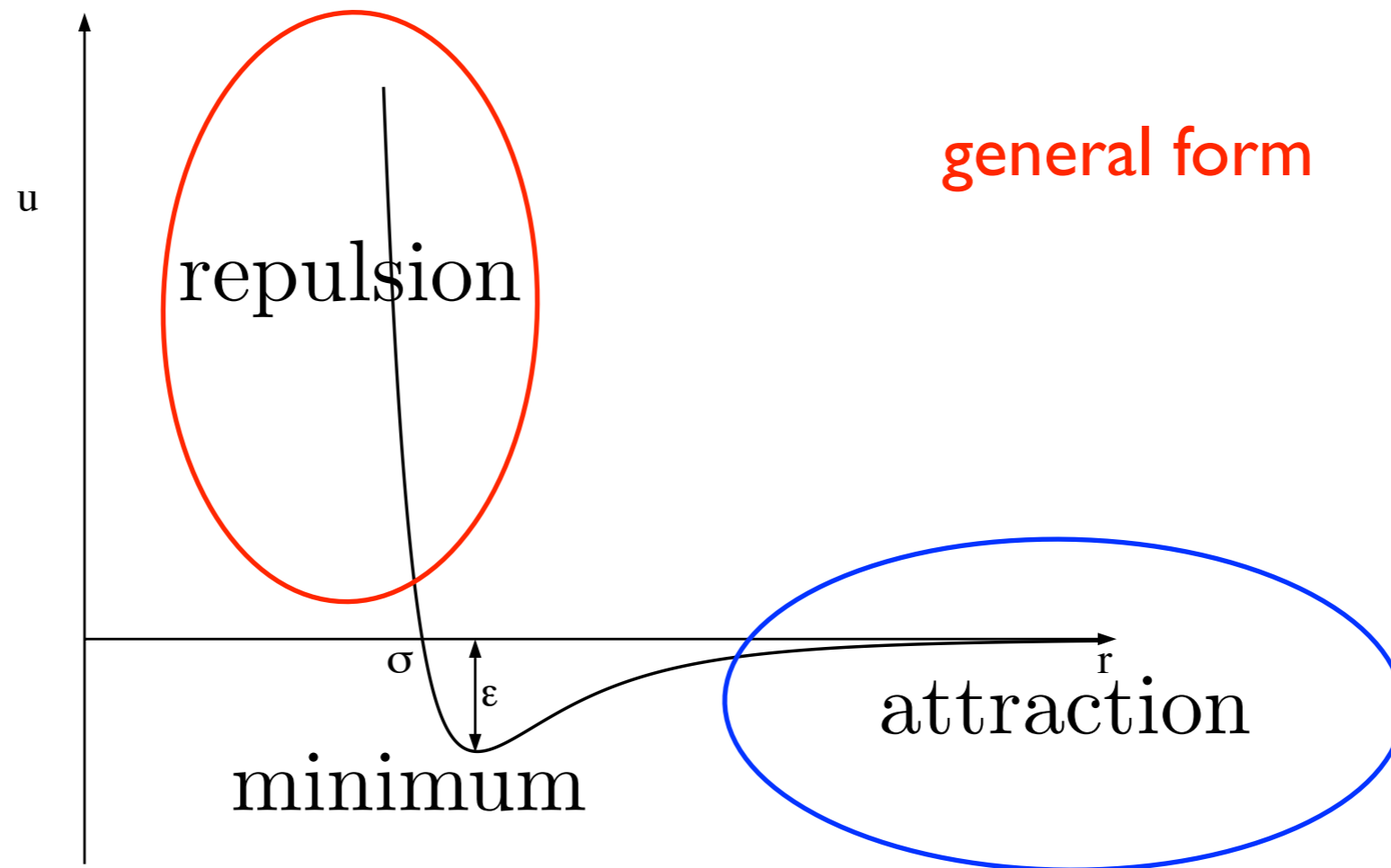
$$\begin{aligned} U &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \phi(\mathbf{r}(\mathbf{R}) - \mathbf{r}(\mathbf{R}')) = \\ &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \phi(\mathbf{R} - \mathbf{R}' + \mathbf{u}(\mathbf{R}) - \mathbf{u}(\mathbf{R}')) \end{aligned}$$

In general, an “effective” potential between two atoms or molecules is different from the “bare” potential between them!



x

A typical 2-body effective potential



a strong repulsion for small r and a weak attraction at large r .

consequence of the Pauli exclusion principle.
core repulsion

x

mutual polarization of each molecule;
van der Waals

$$\begin{aligned}
 U^{\text{harm}} &= \frac{1}{4} \sum_{\mathbf{R}\mathbf{R}'} [(\mathbf{u}(\mathbf{R}) - \mathbf{u}(\mathbf{R}')) \cdot \nabla]^2 \phi(\mathbf{R} - \mathbf{R}') \\
 &= \frac{1}{4} \sum_{\substack{\mathbf{R}\mathbf{R}' \\ \mu, \nu = x, y, z}} [u_{\mu}(\mathbf{R}) - u_{\mu}(\mathbf{R}')] \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}') [u_{\nu}(\mathbf{R}) - u_{\nu}(\mathbf{R}')]
 \end{aligned}$$

with $\phi_{\mu\nu}(\mathbf{r}) = \frac{\partial^2 \phi(\mathbf{r})}{\partial r_{\mu} \partial r_{\nu}}$

let's rearrange terms in the sum =>

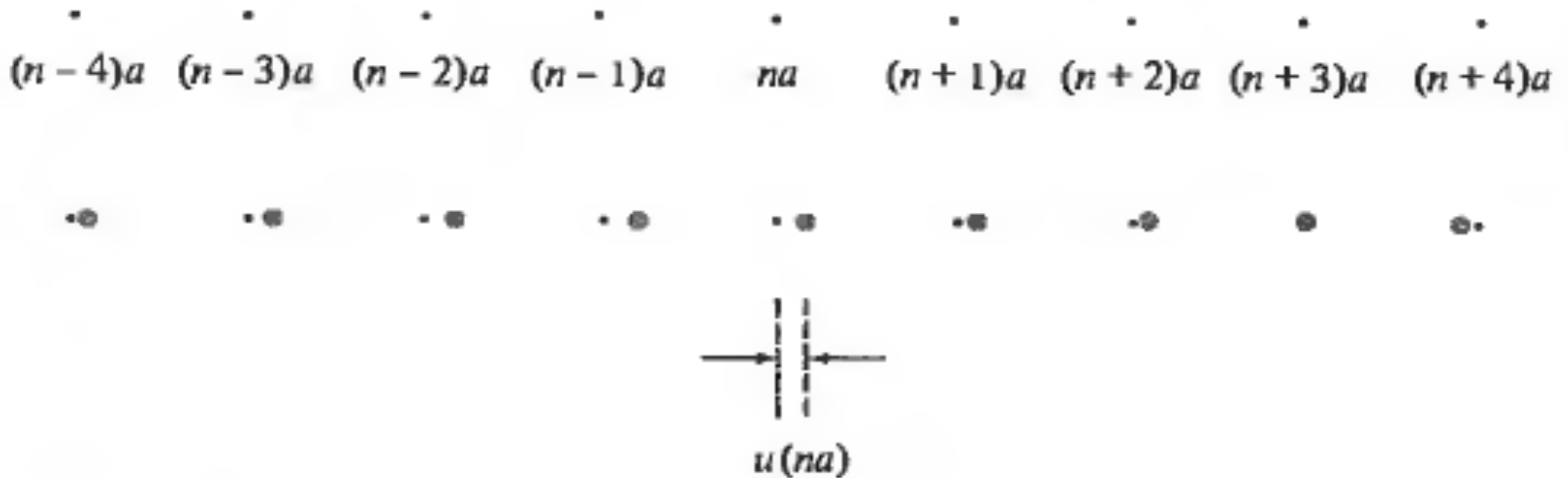
$$\begin{aligned}
 U^{\text{harm}} &= \frac{1}{4} \sum_{\mathbf{R}\mathbf{R}'} [(\mathbf{u}(\mathbf{R}) - \mathbf{u}(\mathbf{R}')) \cdot \nabla]^2 \phi(\mathbf{R} - \mathbf{R}') \\
 &= \frac{1}{4} \sum_{\substack{\mathbf{R}\mathbf{R}' \\ \mu, \nu = x, y, z}} [u_{\mu}(\mathbf{R}) - u_{\mu}(\mathbf{R}')] \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}') [u_{\nu}(\mathbf{R}) - u_{\nu}(\mathbf{R}')]
 \end{aligned}$$

with $\phi_{\mu\nu}(\mathbf{r}) = \frac{\partial^2 \phi(\mathbf{r})}{\partial r_{\mu} \partial r_{\nu}}$

$$= \frac{1}{2} \sum_{\substack{\mathbf{R}\mathbf{R}' \\ \mu\nu}} u_{\mu}(\mathbf{R}) D_{\mu\nu}(\mathbf{R} - \mathbf{R}') u_{\nu}(\mathbf{R}')$$

with $D_{\mu\nu}(\mathbf{R} - \mathbf{R}') = \delta_{\mathbf{R},\mathbf{R}'} \sum_{\mathbf{R}''} \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}'') - \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}')$

normal modes - 1D monoatomic chain (=Bravais lattice)



Suppose only NN interactions

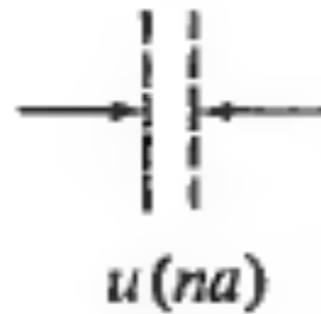
$$U^{\text{harm}} = \frac{1}{2} K \sum_n [u(na) - u([n+1]a)]^2$$

where $K = \phi''(a)$

equivalent model



\cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot
 $(n-4)a$ $(n-3)a$ $(n-2)a$ $(n-1)a$ na $(n+1)a$ $(n+2)a$ $(n+3)a$ $(n+4)a$



$$M\ddot{u}(na) = - \frac{\partial U^{\text{harm}}}{\partial u(na)} = - K[2u(na) - u([n-1]a) - u([n+1]a)]$$

$$M\ddot{u}(na) = -\frac{\partial U^{\text{harm}}}{\partial u(na)} = -K[2u(na) - u([n-1]a) - u([n+1]a)]$$

Apply PBC to a chain of N atoms:

$$u([N+1]a) = u(a); \quad u(0) = u(Na)$$

and seek solutions of the form:

$$u(na, t) \propto e^{i(kna - \omega t)}$$

$$\text{PBC} \Rightarrow e^{ikNa} = 1 \Rightarrow k = \frac{2\pi}{a} \frac{n}{N}$$

(allowed k defined
for $n=0 \dots N-1$ or
 $= -N/2, \dots, N/2$
mod. $2\pi/a$)

Substituting the allowed values of k :

$$\begin{aligned} -M\omega^2 e^{i(kna - \omega t)} &= -K[2 - e^{-ika} - e^{ika}]e^{i(kna - \omega t)} \\ &= -2K(1 - \cos ka)e^{i(kna - \omega t)}, \end{aligned}$$

we have a solution for a given k , provided that $\omega = \omega(k)$, where

$$\omega(k) = \sqrt{\frac{2K(1 - \cos ka)}{M}} = 2\sqrt{\frac{K}{M}} \left| \sin \frac{1}{2}ka \right|.$$

$$\omega(k) = \omega(-k)$$

$$u(na, t) \propto e^{i(kna - \omega t)} \quad \Rightarrow \text{Re or Im}$$

$$u(na, t) \propto \begin{cases} \cos(kna - \omega t) \\ \sin(kna - \omega t) \end{cases}$$

$k, -\omega(k)$ equivalent to $-k, \omega(k)$

$2N$ independent solutions.

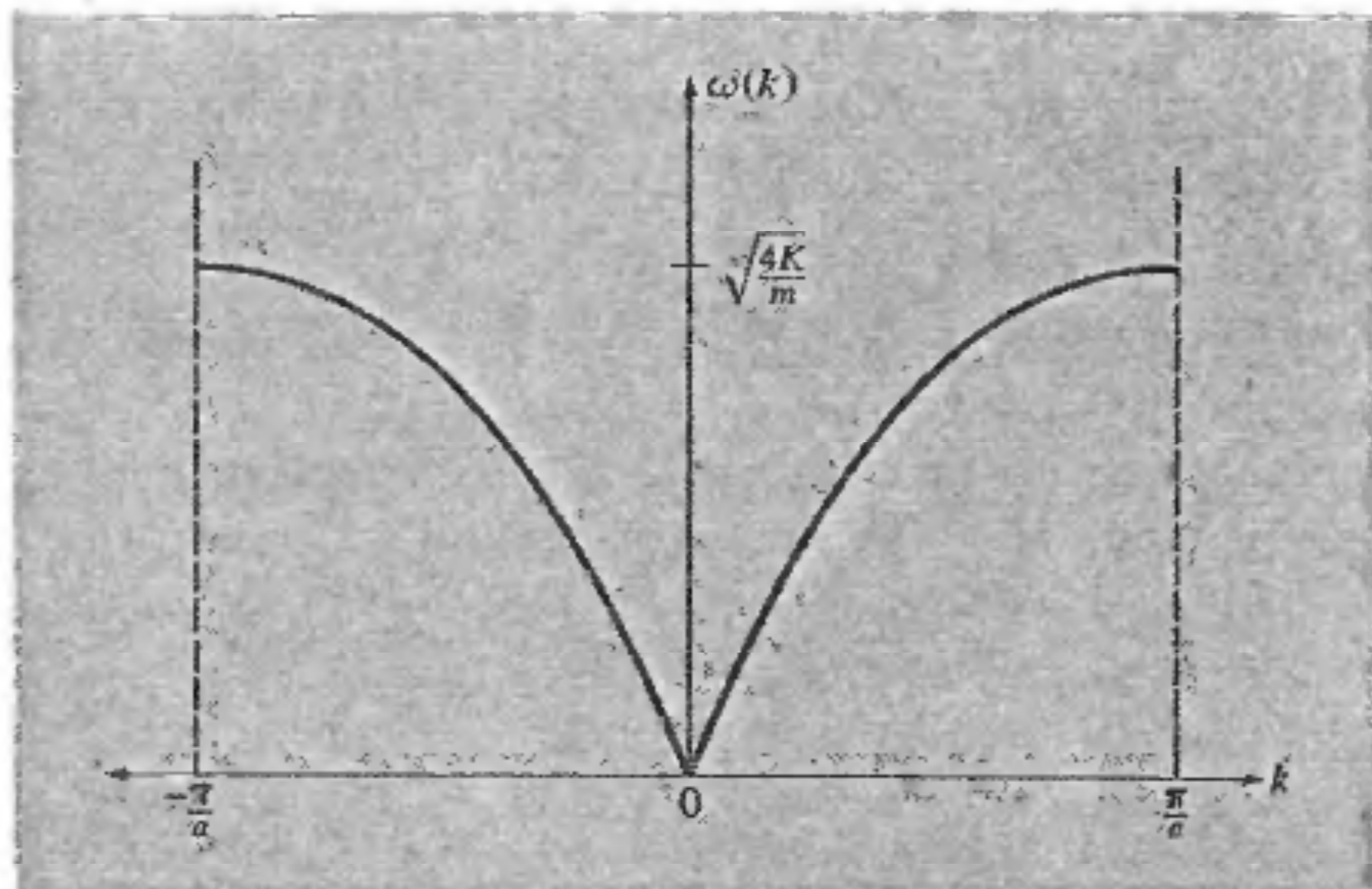
When k is small compared with π/a

ω is linear in k :

$$\omega = \left(a \sqrt{\frac{K}{M}} \right) |k|.$$

Figure 22.8

Dispersion curve for a monatomic linear chain with only nearest-neighbor interactions. Note that ω is linear for small k , and that $\partial\omega/\partial k$ vanishes at the boundaries of the zone ($k = \pm\pi/a$).



Eccitazioni vibrazionali: Fononi in un Reticolo Semplice (monoatomico)

Velocità di propgazione di un onda è: $v_g = d\omega/dK$

A bassa frequenza ($Ka \ll 1$) posso stimare la costante di accoppiamento studiando la **velocità del suono** in un materiale:

$$\omega^2 = (C/M)K^2a^2$$

$$v = \omega/K$$

Velocità del suono tipiche dei materiali sono

Oro: 3240m/s

Alluminio: 6320m/s

Fononi acustici

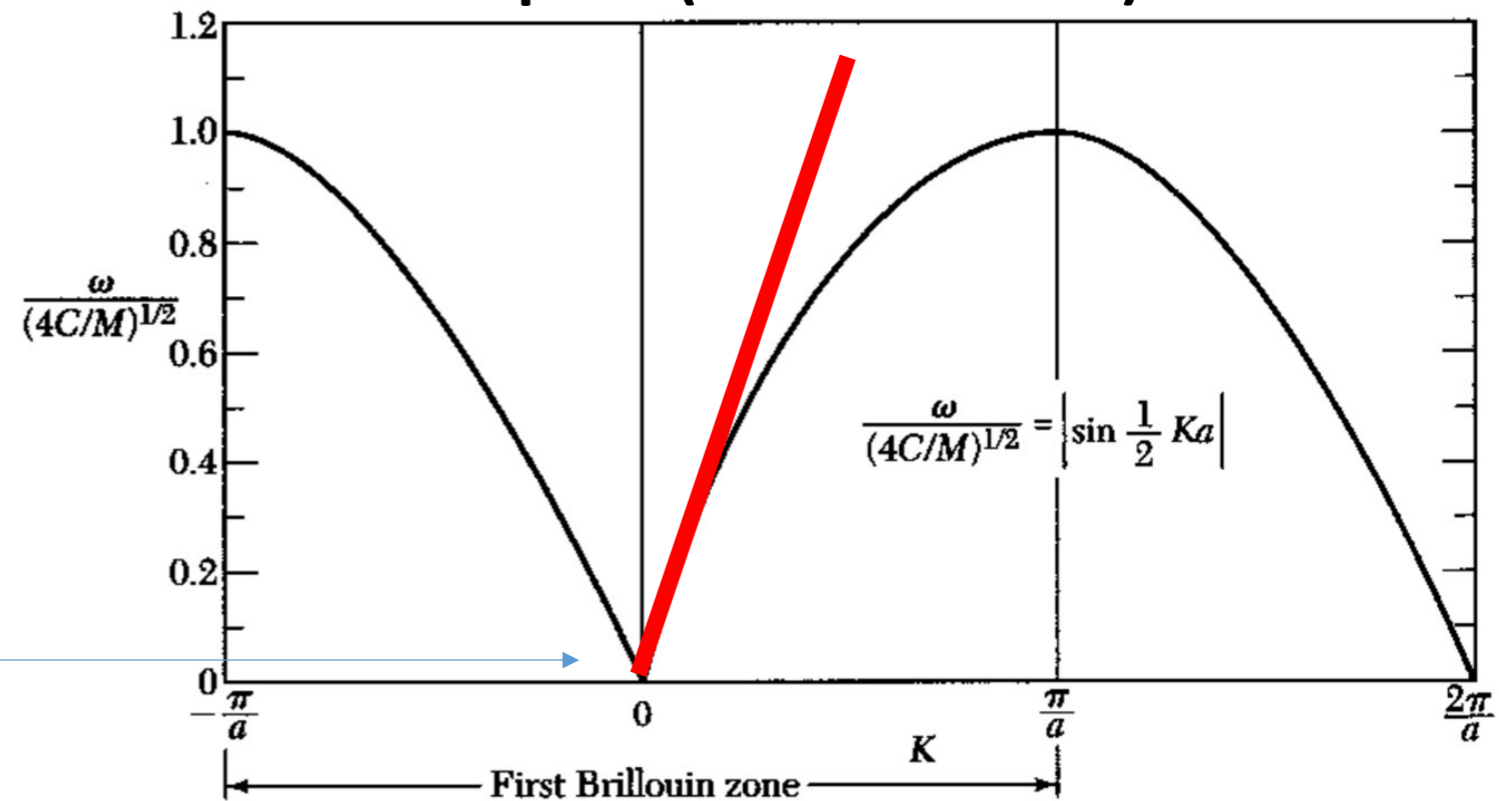
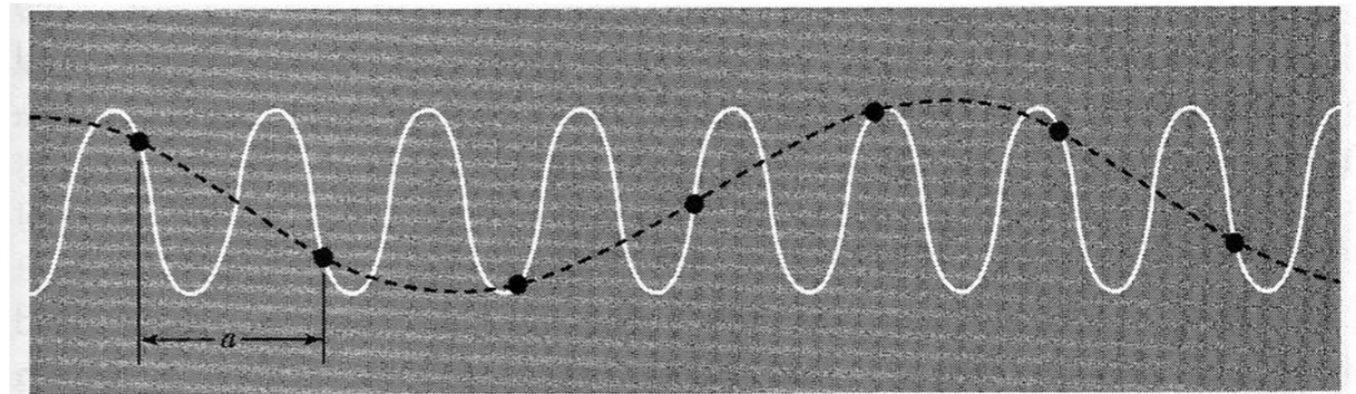


Figure 4 Plot of ω versus K . The region of $K \ll 1/a$ or $\lambda \gg a$ corresponds to the continuum approximation; here ω is directly proportional to K .



(D. Fausti - corso di Struttura - LT Fisica UniTS)

The equations of motion are

$$\begin{aligned} M\ddot{u}_1(na) &= -\frac{\partial U^{\text{harm}}}{\partial u_1(na)} \\ &= -K[u_1(na) - u_2(na)] - G[u_1(na) - u_2([n-1]a)], \\ M\ddot{u}_2(na) &= -\frac{\partial U^{\text{harm}}}{\partial u_2(na)} \\ &= -K[u_2(na) - u_1(na)] - G[u_2(na) - u_1([n+1]a)]. \end{aligned}$$

Apply PBC and seek solutions of the form:

$$\begin{aligned} u_1(na) &= \epsilon_1 e^{i(kna - \omega t)} \\ u_2(na) &= \epsilon_2 e^{i(kna - \omega t)} \end{aligned}$$

=> coupled eqs.

$$\begin{aligned} [M\omega^2 - (K + G)]\epsilon_1 + (K + Ge^{-ika})\epsilon_2 &= 0 \\ (K + Ge^{ika})\epsilon_1 + [M\omega^2 - (K + G)]\epsilon_2 &= 0 \end{aligned}$$

=> impose Det=0

$$[M\omega^2 - (K + G)]^2 = |K + Ge^{-ika}|^2 = K^2 + G^2 + 2KG \cos ka$$

$$\omega^2 = \frac{K + G}{M} \pm \frac{1}{M} \sqrt{K^2 + G^2 + 2KG \cos ka}$$

Figure 22.10

Dispersion relation for the diatomic linear chain. The lower branch is the acoustic branch and has the same structure as the single branch present in the monatomic case (Figure 22.8). In addition, there is now an optical branch (upper branch.)

