

02.04.19

①

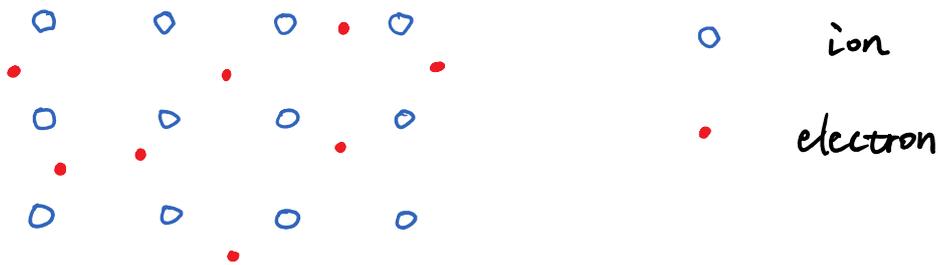
Solid State Theory (SS2019)

Hong-Hao Tu (hong-hao.tu@tu-dresden.de)

Course webpage:

tu-dresden.de/mn/physik/itp/kt/studium/lehre/sst_ss19

Crystal: electrons + ions



Goal: understand electronic / magnetic / optical / thermodynamical properties of solids.

Hamiltonian :

$$H = H_{\text{ion}} + H_{\text{el}} + H_{\text{el-ion}}$$

$$H_{\text{ion}} = \sum_{i=1}^{N_I} \frac{\vec{p}_i^2}{2M_i} + \frac{1}{2} \sum_{i \neq i'}^{N_I} \underbrace{V(\vec{R}_i - \vec{R}_{i'})}_{\parallel \frac{z_i z_{i'} e^2}{4\pi\epsilon_0 |\vec{R}_i - \vec{R}_{i'}|}}$$

$$H_{\text{el}} = \sum_{j=1}^{N_e} \frac{\vec{p}_j^2}{2m} + \frac{1}{2} \sum_{j \neq j'}^{N_e} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_j - \vec{r}_{j'}|}$$

$$H_{\text{el-ion}} = - \sum_{i=1}^{N_I} \sum_{j=1}^{N_e} \frac{z_i e^2}{4\pi\epsilon_0 |\vec{R}_i - \vec{r}_j|}$$

$$H \psi(\vec{r}_1, \dots, \vec{r}_{N_e}; \vec{R}_1, \dots, \vec{R}_{N_I}) = E \psi(\vec{r}_1, \dots, \vec{r}_{N_e}; \vec{R}_1, \dots, \vec{R}_{N_I})$$

too difficult to solve !

$$N_e, N_I \sim 10^{23}$$

Ideas for simplification :

- 1) Symmetries (e.g. translation, lattice, spin...)
- 2) Separation of degrees of freedom (d.o.f.)
- 3) Energy scales

§1. Lattice dynamics

$$M_{\text{ion}} \gg M_e \quad (M_{\text{proton}} \approx M_{\text{neutron}} \approx 1836 M_e)$$

↳ "slow dynamics!"

Imagine that electrons stay in the ground state:

$$H_{\text{ion}} = \sum_{i=1}^{N_I} \frac{\vec{p}_i^2}{2M_i} + \frac{1}{2} \sum_{i \neq i'}^{N_I} V(\vec{R}_i - \vec{R}_{i'})$$

$$+ \underbrace{\mathcal{E}_{\text{el-ion}}(\{\vec{R}_i\})}_{\parallel}$$

$$\langle \mathcal{H}_{\text{el-ion}} \rangle_{\text{el}} = - \sum_{i=1}^{N_I} \sum_{j=1}^{N_e} \frac{z_i e^2}{4\pi\epsilon_0} \left\langle \frac{1}{|\vec{R}_i - \vec{r}_j|} \right\rangle_{\text{el}}$$

$\mathcal{H}_{\text{el-ion}}$ provides a "background" potential for ions.

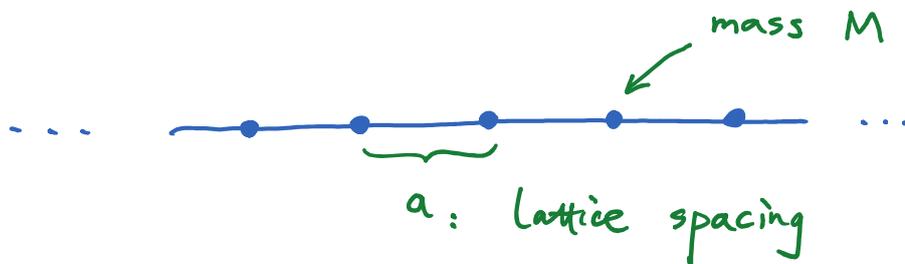
(More rigorous treatment: Born-Oppenheimer approximation)

simpler than before, but still difficult to solve!

Let's first get some intuitions from the classical limit.

* Classical theory of lattice vibrations

- 1D monoatomic chain



equilibrium position: ja $j=1, 2, \dots, N$

displacement: $u_j \Rightarrow R_j = ja + u_j$

physical requirement: $|u_j| \ll a$

(otherwise the crystal would melt)

$$H = \sum_{i=1}^N \frac{1}{2} M \dot{u}_i^2 + V(\{u_i\})$$

$$V(\{u_i\}) \stackrel{|u_i| \ll a}{=} V_0 + \sum_{i=1}^N \underbrace{\left(\frac{\partial V}{\partial u_i} \right) \Big|_0}_{=0} u_i + \frac{1}{2} \sum_{i,j=1}^N \left(\frac{\partial^2 V}{\partial u_i \partial u_j} \right) \Big|_0 u_i u_j$$

evaluated at $u_j=0$

$+ O(u^3)$ (equilibrium position minimizes V)

dropped \Rightarrow harmonic approximation

$$D_{ij} \equiv \left(\frac{\partial^2 V}{\partial u_i \partial u_j} \right) \Big|_0 = D_{ji} \quad (D \text{ real})$$

D : $N \times N$ symmetric matrix, called dynamical matrix

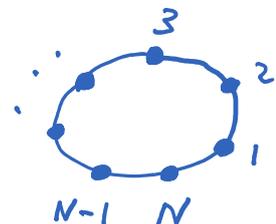
Force acting on the i -th ion:

$$\begin{aligned} F_i &= - \frac{\partial V}{\partial u_i} \\ &= - \frac{\partial}{\partial u_i} \left(V_0 + \frac{1}{2} \sum_{j,l=1}^N D_{jl} u_j u_l \right) \\ &= - \sum_{j=1}^N D_{ij} u_j \end{aligned}$$

Periodic boundary condition (PBC): $u_{j+N} = u_j$

(translation symmetry imposed)

Further constraints on D_{ij} :



$$D_{i+l, j+l} = D_{ij} \equiv D_{j-i} \quad (\text{translation symmetry})$$

$$\sum_{j=1}^N D_{ij} = 0 \quad (\text{global shift: } u_j = u \neq 0 \quad \forall j)$$

no force: $0 = F_i = -u \sum_{j=1}^N D_{ij}$

Classical equation of motion (E.O.M.):
(Newton's second law)

$$M\ddot{u}_i = F_i = -\sum_{j=1}^N D_{ij} u_j$$

Solution: $u_i = A_i e^{-i\omega t}$
↪ time independent

$$\Rightarrow -M\omega^2 A_i \cancel{e^{-i\omega t}} = -\sum_{j=1}^N D_{ij} A_j \cancel{e^{-i\omega t}}$$

(Linear equations determining A_j)

$$A_j = A e^{i\varphi_j a}$$

$$\Rightarrow M\omega^2 \cancel{A} e^{i\varphi_j a} = \sum_{l=1}^N D_{jl} \cancel{A} e^{i\varphi_l a}$$

Dispersion relation:

$$\omega_q = \sqrt{\frac{1}{M} \sum_{l=1}^N D_{jl} e^{i\varphi(l-j)a}} = \sqrt{\frac{D(q)}{M}}$$

$$D(q) \equiv \sum_{\delta} D_{\delta} e^{i\varphi\delta}$$

translation symmetry
 $D_{jl} = D_{l-j} \equiv D_{\delta}$

02.04.19

⑦

Lattice vibration takes the form of a running wave:

$$\begin{aligned}
 u_j(t) &= A_j e^{-i\omega t} \\
 &= A e^{i(qja - \omega t)}
 \end{aligned}$$

↘ amplitude

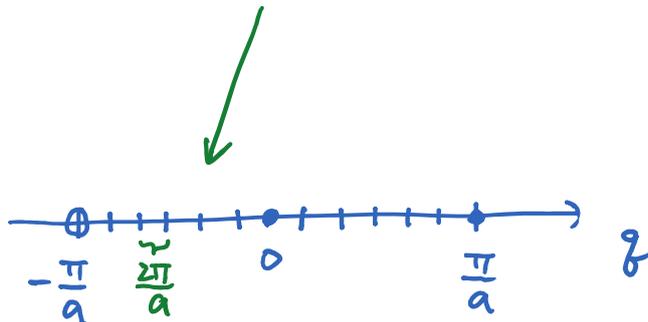
Periodic boundary imposes constraint on q :

$$u_{j+N} = u_j \Rightarrow e^{iqNa} = 1$$

$$q = 0, \pm \frac{2\pi}{Na}, \pm \frac{4\pi}{Na}, \dots, \pm \frac{(N-2)\pi}{Na}, \frac{\pi}{a} \quad (N \text{ even})$$

$$q \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

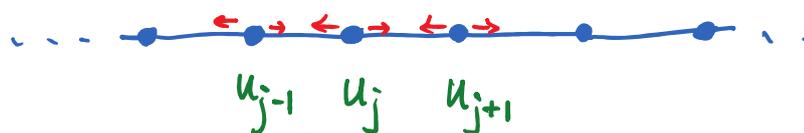
first Brillouin zone (FBZ)



$$q = -\frac{\pi}{a} \text{ is equivalent to } q = \frac{\pi}{a}.$$

(They differ only by a reciprocal vector $\frac{2\pi}{a}$.)

Example: nearest-neighbor interactions



Nonvanishing D_{ij} :

$$\begin{cases} D_{jj} = 2c \\ D_{j-1,j} = D_{j+1,j} = -c \end{cases}$$

$$\begin{aligned} V(\{u_j\}) &= V_0 + \frac{1}{2} \sum_{i,j} D_{ij} u_i u_j \\ &= V_0 + \frac{1}{2} c \sum_{j=1}^N (-u_{j-1} u_j + 2u_j^2 - u_{j+1} u_j) \\ &= V_0 + \frac{1}{2} c \sum_{j=1}^N \underbrace{(u_j - u_{j+1})^2}_{\text{coupled springs}} \end{aligned}$$

coupled springs

$$M \ddot{u}_j = - \sum_{l=1}^N D_{jl} u_l = -c (2u_j - u_{j+1} - u_{j-1})$$

Solution: $u_j(t) = A e^{iqaj - i\omega t}$

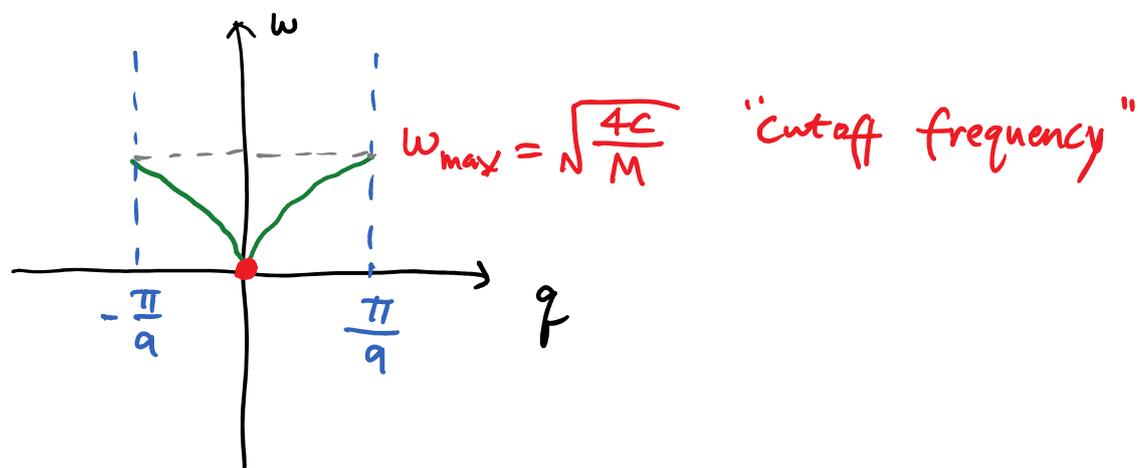
Dispersion: $\omega(q) = \sqrt{\frac{D(q)}{M}}$

$$\begin{aligned} D(q) &= \sum_{\delta=\pm 1,0} D_{\delta} e^{iqa\delta} = 2c - ce^{iqa} - ce^{-iqa} \\ &= 2c (1 - \cos qa) = 4c \sin^2 \frac{qa}{2} \end{aligned}$$

02.04.19

(9)

$$\Rightarrow \omega(q) = \sqrt{\frac{4c}{M}} \left| \sin \frac{qa}{2} \right|$$



Key feature: $\omega_q \rightarrow 0$ for $q \rightarrow 0$ (long wavelength limit)

$$\omega_q \approx v_s |q|, \quad v_s = \sqrt{\frac{c}{M}} a \quad (\text{sound velocity})$$

Estimation of cutoff frequency:

$$\omega_{\max} = \sqrt{\frac{4c}{M}} = \frac{2v_s}{a} \approx \frac{10^3 \text{ m/s}}{10^{-10} \text{ m}} = 10^{13} \text{ Hz}$$

Continuum limit ($|q| \rightarrow 0$, wavelength $\gg a$):

$$u_{j+1} - u_j \approx a \frac{\partial u}{\partial x} + \frac{1}{2} a^2 \left(\frac{\partial^2 u}{\partial x^2} \right) + \dots$$

$$\Rightarrow M \ddot{u} = C a^2 \frac{\partial^2 u}{\partial x^2}$$

elastic wave with velocity $v_s = \sqrt{\frac{c}{M}} a$!