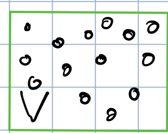
Recall Lecture I

INTRO: MANY-BODY PROBLEM (IN EQUILIBRIUM)

$N \simeq 10^{23}$ particles at fixed (say) (T, V) $\quad$ $(N \gg 1 \longrightarrow N \to \infty)$

Microscopic description $\hat{H}(\{\hat{r}_i, \hat{p}_i\}_{i=1}^{N})$ $\longrightarrow$ Macroscopic description

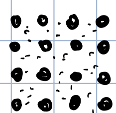
T 

$p(T,V,N)$, $\vec{j}(T,V,N,\vec{E})$, ...

(thermodynamic and transport properties)

EXAMPLE (PROTOTYPE) MANY-BODY HAMILTONIAN

lattice of ions + electrons $\qquad$ e.g. metallic material



$$H_e = \sum_i \frac{\bar{p}_i^2}{2m} + \sum_{i<j} V_{ee}(\bar{r}_i - \bar{r}_j)$$

$$H_i = \sum_I \frac{\bar{P}_I^2}{2M} + \sum_{I<J} V_{ii}(\bar{R}_J - \bar{R}_I)$$

$$H_{ei} = \sum_{i,I} V_{ei}(\bar{R}_I - \bar{r}_i)$$

$$H = H_e + H_i + H_{ei}$$

(certain elements, e.g. lattice structure put in "by hand").

- Not fully realistic (spin, impurities ...)
- Valid only down to some length scale (e.g. does not resolve ions' structure)
- Valid only up to some energy scale (too high T $\to$ lattice melts...)

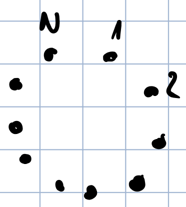
$\to$ "Ab initio" approaches (take H as it is...) $\longrightarrow$ numerics

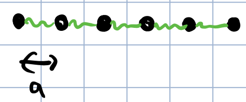
$\to$ Simplify the model to capture most essential elements related to certain phenomenology

Today: Physics of lattice vibrations (ions only)

"Prototype crystal"

$d=1$ (more general case later on)





• Periodic B.C

$L = Na$

R_j - position of the j-th atom

$R_{N+1} = R_1$

Hamiltonian

• $T = \sum_{j=1}^{N} \frac{p_j^2}{2m}$

$N \gg 1 \qquad N \approx 10^{23}$

• $V = \sum_{j=1}^{N} \frac{k_s}{2}(R_{j+1} - R_j - a)^2$ (coupled harmonic oscillators)

→ only nearest-neighbours interact.

$$H = \sum_{j=1}^{N}\left(\frac{p_j^2}{2m} + \frac{k_s}{2}(R_{j+1} - R_j - a)^2\right)$$

→ small deviations from eq. positions.

$$R_j = \underbrace{\bar{R}_j}_{\parallel \; ja} + \phi_j$$

$$H = \sum_{j=1}^{N}\left(\frac{p_j^2}{2m} + \frac{m\omega^2}{2}(\phi_{j+1} - \phi_j)^2\right)$$

$\omega^2 := \frac{k_s}{m}$

Translation symmetry
$$\left.\begin{array}{l} p_j \to p_{j+1} \\ \phi_j \to \phi_{j+1} \end{array}\right\} \text{H does not change.}$$

Fourier transform (discrete)

$$\{\phi_j\}_{j=1}^{N} \longmapsto \{\phi_q\}_{q=1}^{N}$$

$$\{p_j\}_{j=1}^{N} \longmapsto \{p_q\}_{q=1}^{N}$$

$$\begin{cases} \phi_j = \frac{1}{\sqrt{N}} \sum_q e^{iqR_j} \phi_q \\ p_j = \frac{1}{\sqrt{N}} \sum_q e^{iqR_j} p_q \end{cases}$$

$R_j = aj$!

PBC $\quad \phi_{j+N} = \phi_j \quad \rightarrow \quad e^{iqNa} = 1 \quad e^{iqL} = 1 \quad qL = 2\pi n$

$$q = \frac{2\pi}{L} n$$

$$n \in \{0, 1, 2 \dots N-1\} \rightarrow q \geq 0 \quad q < \frac{2\pi}{a}$$

$$q \in \left[0, \frac{2\pi}{a}\right[$$

another choice $\quad q \in \left]-\frac{\pi}{a}, \frac{\pi}{a}\right]$

(standard choice)

Moreover: $\displaystyle \frac{1}{N}\sum_{j=1}^{N} e^{i(q_1 - q_2)R_j} = \delta_{q_1 q_2}$

Inverse transform: $\begin{cases} \phi_q = \dfrac{1}{\sqrt{N}} \displaystyle\sum_j e^{-iqR_j} \phi_j \\ p_q = \dfrac{1}{\sqrt{N}} \displaystyle\sum_j e^{-iqR_j} p_j \end{cases}$ $\quad (*)$

$\begin{cases} \phi_q^* = \phi_{-q} \\ p_q^* = p_{-q} \end{cases}$ $(\phi_j, p_j \text{ real})$ $\quad \begin{cases} \phi_q^+ = \phi_{-q} \\ p_q^+ = p_{-q} \end{cases}$ $(\phi_j, p_j \text{ hermitian})$

classical variant $\qquad$ quantum variant

Plug ϕ_j, p_j into H

- $\displaystyle \sum_{j=1}^{N} \frac{p_j^2}{2m} = \frac{1}{2m}\sum_{j=1}^{N}\frac{1}{N}\sum_q\sum_{q'} e^{iqR_j} e^{iq'R_j} p_q p_{q'} = \frac{1}{2m}\sum_q\sum_{q'} p_q p_{q'} \delta_{q,-q'} =$
$$= \frac{1}{2m}\sum_q p_q p_{-q}$$

- $\displaystyle \sum_{j=1}^{N}(\phi_j - \phi_{j+1})^2 = \sum_{j=1}^{N}\left(\phi_j\phi_j - \phi_j\phi_{j+1} - \phi_{j+1}\phi_j + \phi_{j+1}\phi_{j+1}\right) =$
$$= \sum_{j=1}^{N}\left(2\phi_j\phi_j - \phi_j\phi_{j+1} - \phi_j\phi_{j-1}\right) =$$
$$= \sum_{j=1}^{N}\phi_j\left(2\phi_j - \phi_{j+1} - \phi_{j-1}\right) =$$

$$= \sum_{j=1}^{N} \frac{1}{N} \sum_q e^{iqR_j} \phi_q \sum_{q'} \left(2 e^{iq'R_j} \phi_{q'} - e^{iq'R_j} e^{iq'a} \phi_{q'} - e^{iq'R_j} e^{-iq'a} \phi_{q'} \right) \quad (4)$$

$$= \frac{1}{N} \sum_q \sum_{q'} \phi_q \phi_{q'} \underbrace{\sum_j e^{i(q+q')R_j}}_{N \delta_{q,-q'}} \underbrace{\left(2 - e^{iq'a} - e^{-iq'a} \right)}_{2(1-\cos q'a) = 2\left(1 - \cos^2\frac{q'a}{2} + \sin^2\frac{q'a}{2}\right) = 4\sin^2\frac{q'a}{2}}$$

$$= \sum_q 4 \sin^2 \frac{qa}{2} \phi_q \phi_{-q}$$

$$H = \sum_q \left(\frac{1}{2m} p_q p_{-q} + \underbrace{\frac{m\omega^2}{2} 4 \sin^2 \frac{qa}{2}}_{\frac{m}{2}\omega_q^2} \phi_q \phi_{-q} \right)$$

$$\omega_q := 2\omega \left| \sin \frac{qa}{2} \right|$$

$$H = \sum_q \left(\frac{1}{2m} p_q p_{-q} + \frac{m\omega_q^2}{2} \phi_q \phi_{-q} \right)$$

$$H = \sum_{q \neq 0} \left(\frac{1}{2m} p_q p_{-q} + \frac{m\omega_q^2}{2} \phi_q \phi_{-q} \right) + \underbrace{\frac{1}{2m} p_0^2}_{H_0}$$

(uniform motion of the entire system).

Recall oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

introduce

$$\begin{cases} a_q := \sqrt{\frac{m\omega_q}{2\hbar}} \left(\phi_q + \frac{i}{m\omega_q} p_q \right) \\ a_q^+ := \sqrt{\frac{m\omega_q}{2\hbar}} \left(\phi_{-q} - \frac{i}{m\omega_q} p_{-q} \right) \end{cases}$$

inverting

$$\begin{cases} \phi_q = \sqrt{\frac{\hbar}{2m\omega_q}} \left(a_q + a_{-q}^+ \right) \\ p_q = -i \sqrt{\frac{m\omega_q\hbar}{2}} \left(a_q - a_{-q}^+ \right) \end{cases}$$

Plug into H.

$$H = H_0 + \sum_{q\neq 0}\left(\frac{1}{2\cancel{m}}\frac{\cancel{m}\omega_q\hbar}{2}(-1)\left(a_q - a_{-q}^\dagger\right)\left(a_{-q} - a_q^\dagger\right) + \frac{\cancel{m}\omega_q^{\cancel{2}}}{2}\frac{\hbar}{2\cancel{m}\cancel{\omega_q}}\left(a_q + a_{-q}^\dagger\right)\left(a_{-q} + a_q^\dagger\right)\right)$$

$$H = H_0 + \frac{1}{4}\sum_{q\neq 0}\hbar\omega_q\left(\cancel{-a_q a_{-q}} + a_q a_q^\dagger + a_{-q}^\dagger a_{-q} - \cancel{a_{-q}^\dagger a_q^\dagger} + \cancel{a_q a_{-q}} + a_q a_q^\dagger + a_{-q}^\dagger a_{-q} + \cancel{a_{-q}^\dagger a_q^\dagger}\right)$$

$$= H_0 + \frac{1}{2}\sum_{q\neq 0}\hbar\omega_q\left(a_q a_q^\dagger + a_q^\dagger a_q\right) = H_0 + \frac{1}{2}\sum_{q\neq 0}\hbar\omega_q\left(2a_q^\dagger a_q + [a_q, a_q^\dagger]\right)$$

Specify to quantum case.

$$[\phi_q, p_{q'}] = \frac{1}{N}\sum_{jj'} e^{-i(qR_j + q'R_{j'})}\underbrace{[\phi_j, p_{j'}]}_{i\hbar\delta_{j,j'}} = \frac{i\hbar}{N}\sum_j e^{-i(q+q')R_j} = i\hbar\,\delta_{q,-q'}$$

$$[a_q, a_{q'}^\dagger] = \frac{m}{2\hbar}\sqrt{\omega_q\omega_{q'}}\left\{\overbrace{[\phi_q, \phi_{-q'}]}^{=0} - \frac{i}{m\omega_{q'}}\overbrace{[\phi_q, p_{-q'}]}^{i\hbar\delta_{q,q'}} + \frac{i}{m\omega_q}\overbrace{[p_q, \phi_{-q'}]}^{-i\hbar\delta_{q,q'}} + \frac{1}{m^2\omega_q\omega_{-q}}\underbrace{[p_q, p_{-q'}]}_{0}\right\} =$$

$$= \frac{m}{2\hbar}\omega_q\left(\frac{\hbar}{m\omega_q}\cdot 2\,\delta_{q,q'}\right) = \delta_{q,q'}$$

$$[a_q, a_{q'}^\dagger] = \delta_{q,q'}$$

$$H = H_0 + \sum_{q\neq 0}\hbar\omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right)$$