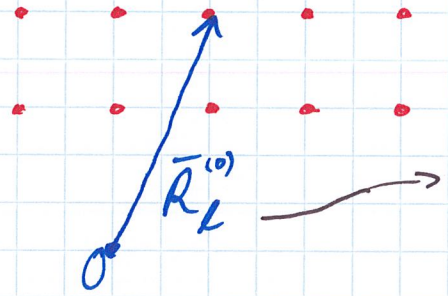
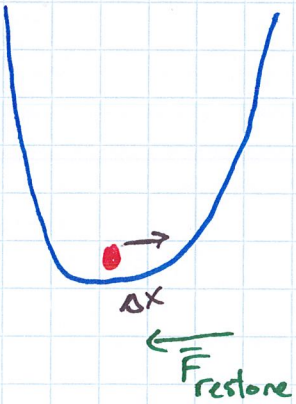
The Dynamic Lattice

Until now, we have only considered a static lattice. That is, an unchanging or ridgid Bravais Lattice



→ position of the ℓ^{th} Bravais Lattice pt. (atom or ion)

Each atom is actually in a deep potential well which "holds" it in place.



→ the atom can move out of it's equilibrium position

→ but as it does, it experiences a restoring force which drives it back towards $\bar{R}_\ell^0$

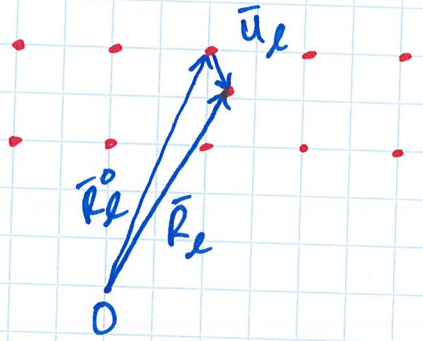
- If the restoring forces are large, the ion can only move a small distance from its equil. position:

$$\bar{R}_\ell = \bar{R}_\ell^0 + \bar{u}_\ell$$

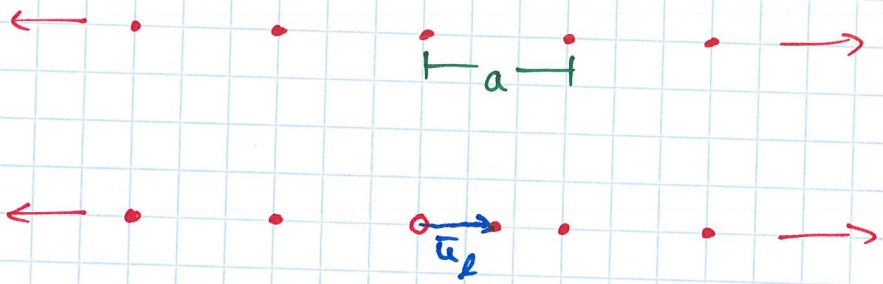
$\bar{R}_\ell$ → position of ion ℓ

$\bar{R}_\ell^0$ → equil. position

$\bar{u}_\ell$ → displacement of ℓ from equil.



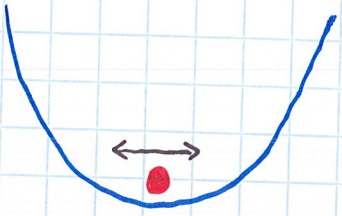
1D chain of atoms



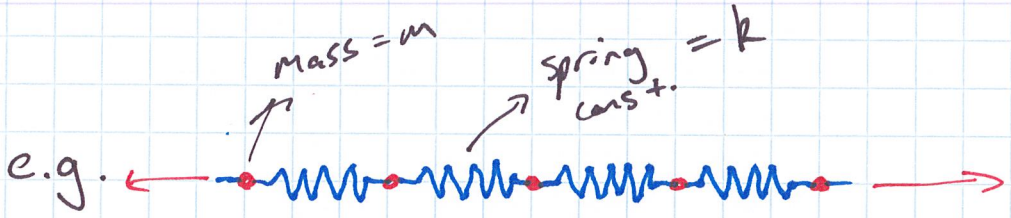
$$\bar{R}_\ell = \bar{R}^\circ_\ell + \bar{u}_\ell = a\ell + u_\ell$$

At low temperatures u_ℓ is small. But as T increases u_ℓ may grow to $\approx a$, at which point there is no longer a meaningful crystal, just an amorphous collection of atoms.

$\Rightarrow$ Melting point



- well below the melting point the displacement of atoms (u_ℓ) leads to coupled harmonic motion



→ a chain of masses connected by springs.

Note: Adiabatic Approximation

→ can ignore $\bar{e}$ positions when calculating the interaction energy of the ions.

→ $\bar{e}$'s instantaneously "reconfigure" to new atomic positions.

electrons: $v_F \sim 10^8$ cm/s → light & fast

ions: $c_s \sim 10^5$ cm/s → heavy & slow

c_s ↓ speed of sound

Interaction Energy

$$W \equiv W(\bar{R}_1, \ldots \bar{R}_N) \qquad \text{(potential energy)}$$

- interaction energy depends on the positions of the atoms/ions in the lattice (all of them)
- does not depends on $\bar{e}$ positions (explicitly)

Lattice Hamiltonian

$$\mathcal{H} = \sum_{\ell=1}^{N} \frac{P_\ell^2}{2M_\ell} + W(\bar{R}_1, \ldots \bar{R}_N)$$

$\frac{P_\ell^2}{2M_\ell}$: K.E. term for each atoms

$W(\bar{R}_1, \ldots \bar{R}_N)$: interaction of atoms

$P_\ell \rightarrow$ momentum of atom ℓ

$M_\ell \rightarrow$ mass of atom ℓ.

Momentum $\rightarrow$ $P_\ell = M_\ell \dot{R}_\ell = M_\ell \frac{d}{dt}\left[R_\ell^\circ + u_\ell\right]$

$= M_\ell \dot{u}_\ell$ ↳ constant.

$W = W(R_1, \ldots R_N)$

$R_\ell = R_\ell^\circ + u_\ell \rightarrow$ small u_ℓ

Taylor Expand W about equil. positions:

$$W(R_1, \ldots R_N) = W(R_1^\circ, \ldots R_N^\circ) \quad (1)$$

$$+ \sum_\ell \left.\frac{\partial W}{\partial R_\ell}\right|_0 u_\ell \quad (2)$$

$$+ \frac{1}{2} \sum_{\ell,\ell'} \left.\frac{\partial^2 W}{\partial R_\ell \partial R_{\ell'}}\right|_0 u_\ell u_{\ell'} \quad (3) + \ldots\ldots \quad (4)$$

→ eval. @ equil. positions.

(1): $W(R_1^\circ, \ldots R_N^\circ) = 0$ (or a constant)

(2): Note: Force on atom ℓ $\Rightarrow F_\ell = -\dfrac{\partial W}{\partial R_\ell}$

$\therefore \left.\dfrac{\partial W}{\partial R_\ell}\right|_0$ $\Rightarrow$ Force on atom ℓ w all atoms in equil. position...

$= 0$. (No net force @ equilibrium)

(3): 2nd order i.e. Hermonic effects

(4): HOTerms yield anharmonic effects

Define:

$$\varphi^{0}_{\ell,\ell'} \equiv \left.\frac{\partial^2 W}{\partial R_\ell \partial R_{\ell'}}\right|_0$$

Harmonic Lattice Hamiltonian

$$\mathcal{H} = \sum_{\ell} \frac{p_\ell^2}{2M_\ell} + \frac{1}{2}\sum_{\ell,\ell'} \varphi^{0}(\ell,\ell')\, u_\ell u_{\ell'}$$

- unsurprisingly this is looking a lot like a harmonic oscillator

$$\underbrace{\frac{1}{2} m \dot{x}^2}_{\text{K.E.}} + \underbrace{\frac{1}{2} k x^2}_{\text{Potential energy}}$$

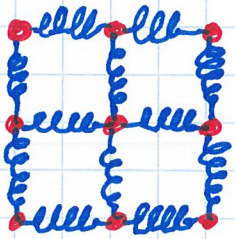
$k \rightarrow$ force const. of spring.

$$\Rightarrow \varphi^{0}(\ell,\ell') \equiv \frac{\partial^2 W}{\partial R_\ell \partial R_{\ell'}} = \text{Force constant}$$

- Not a system of N independent oscillators
- Instead, N-coupled harmonic oscillators
- "Normal modes" => coupled oscillators

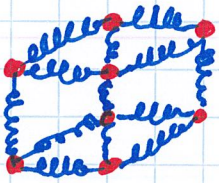
1D, N atoms

N normal modes



2D, N atoms

2N normal modes



3D, N atoms

3N normal modes

"Ball & Spring Analogy"

What is $\Phi^\circ(\ell,\ell')$? Force constant ... of what?

→ Force on atom ℓ (@ equil. position R°_ℓ) due to displacement of atom ℓ', w all other atoms @ equil.

Recall: $F_\ell = \dfrac{\partial W}{\partial R_\ell}$ General config: $W = W(\bar{R}_1 \ldots \bar{R}_N)$

$$= \frac{\partial}{\partial R_\ell} W(R_1, \ldots R_{\ell-1}, R_\ell, R_{\ell+1}, \ldots R_N)$$

Take all atoms to be in equil. except ℓ'

$R_{l'} = R^0_{l'} + u_{l'}$

$$F = \frac{\partial}{\partial R_l} W(R^0_1, \dots R^0_{l'-1}, R_{l'}, R^0_{l'+1}, \dots R^0_N)$$

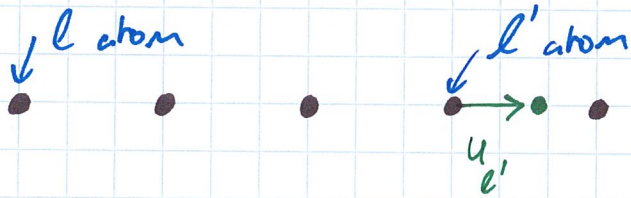
Taylor Exp about equil. positions:

$$F = \frac{\partial}{\partial R_l} W(R^0_1 \dots, R_{l'}, \dots R_l, \dots R^0_N)\Big|_0$$

$$\approx \frac{\partial W}{\partial R_l}\Big|_{R_l = R^0_l} \to 0 \quad + \frac{\partial^2 W}{\partial R_{l'} \partial R_l}\Big|_0 u_{l'} + \dots$$

i.e. For unit displacement of $u_{l'}$:

$$F_l = \varphi^0(l, l') = \frac{\partial^2 W}{\partial R_{l'} \partial R_l}\Big|_0$$



→ displacement of atom l' by $u_{l'}$

→ induces force on atom l of $\varphi^0(l, l') u_{l'}$
(assuming l in equil. position).