CHAIN OF ATOMS – STRING – QUANTIZATION

A. Altland & B. Simons, Condensed Matter Field Theory, pp. 3–24

Coulomb forces between ions

Ion coordinate R_i

At $T=0$ in equilibrium $\boxed{R_i = a\,i = \bar{R}_i}$

Low energy problem $\leftrightarrow$ harmonic oscillator

$V(x) = V(x_0) + \underbrace{V'(x_0)}_{\text{extremum}\ \Vert\ 0}(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2$

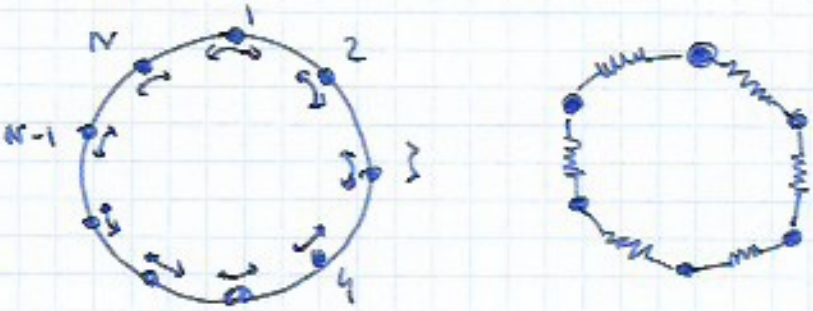
$$\boxed{\hat{H} = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m} + \frac{k}{2}\left(R_{i+1} - R_i - a\right)^2\right]}$$

+ periodic boundary conditions

$R_1 \equiv R_{N+1}$

$L = aN$

$\uparrow$ circumference



Firstly we will construct classical field theory (continuous mechanics) of this system in thermodynamic limit

Lagrangian

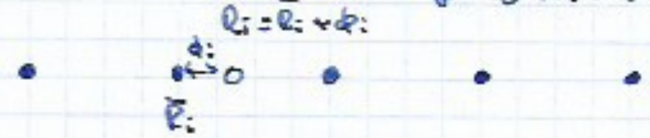
$$\boxed{L = T - V = \sum_{i=1}^{N}\left[\frac{m\dot{R}_i^2}{2} - \frac{k_0}{2}\left(R_{i+1} - R_i - a\right)^2\right]}$$

$\dot{R}_i = \frac{dR_i}{dt}$

We consider small vibrations $|R_i(t) - \bar{R}_i| \ll a$

$$\boxed{R_i(t) = \bar{R}_i + \underbrace{\phi_i(t)}_{\text{fluctuation}}} \qquad \text{with } \phi_{N+1}(t) = \phi_1(t)$$

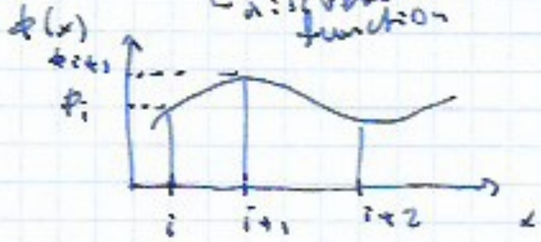
$$|\phi_i(t)| \ll a$$



$$L = \sum_{i=1}^{N} \left[\frac{m}{2} \dot{\phi}_i^{\,2} - \frac{k}{2} (\phi_{i+1} - \phi_i)^2 \right]$$

Continuum limit $\quad N \simeq 10^{23} \to \infty, \quad L \to \infty, \quad a \to 0$

$$i = 1, 2, \dots, N, \quad \underbrace{\phi_i}_{\text{discrete function}} \longleftrightarrow \underbrace{\phi(x)}_{\text{smooth function}} \qquad x \in [0, L]$$



We define $\qquad [\sqrt{a}] = [\sqrt{m}]$

$$\phi_i \to \sqrt{a}\, \phi(x)\big|_{x = ai} \quad \Rightarrow \quad [\phi_i] = [m] \text{ and } [\phi(x)] = [\sqrt{m}]$$

$$\phi_{i+1} - \phi_i \to \frac{\phi(x+a) - \phi(x)}{a} \sqrt{a} \cdot a \xrightarrow[a \to 0]{} \left(\partial_x \phi(x)\big|_{x = ai} \right) \cdot a^{3/2}$$

$$\sum_{i=1}^{N} (\,) = \frac{1}{a} \sum_{i=1}^{N} a\,(\,) \xrightarrow[a \to 0]{} \frac{1}{a} \int_0^L dx\,(\,) \qquad L = aN$$

Now,

$$L = \frac{1}{a} \int_0^L dx \left[\frac{ma}{2} (\dot{\phi}(x))^2 - \frac{k}{2} (\partial_x(x))^2 \cdot a^3 \right]$$

$$\Rightarrow \boxed{L = \int_0^L dx \left[\frac{m}{2} (\dot{\phi}(x))^2 - \frac{\underbrace{ka^2}_{\text{new coupling constant (renormalized)}}}{2} (\partial_x \phi(x))^2 \right]} \qquad ka^2 \xrightarrow[a \to 0]{} \text{const.}$$

$[L] = [J]$

Lagrangian density $\quad \mathcal{L}[\phi, \partial_x \phi, \dot{\phi}] = \frac{m}{2} \dot{\phi}(x)^2 - \frac{ka^2}{2} (\partial_x \phi(x))^2$

$$[\mathcal{L}] = [J/m]$$

classical action

$$S[\varphi] = \int dt \; L[\varphi] = \int dt \int dx \; \mathcal{L}[\varphi, \partial_x \varphi, \partial_t \varphi]$$

Equation of motion – principle of minimal action

$$\varphi(x,t) \to \Phi(x,t) + \varepsilon\, \eta(x,t)$$

$\uparrow$ classical part

[small fluctuations | variations

$$\delta S[\varphi] = 0$$

fixed boundaries

$$\delta S[\varphi] = S[\Phi + \varepsilon\eta] - S[\Phi] = 0 + \mathcal{O}(\varepsilon^2)$$

$$S[\Phi+\varepsilon\eta] = S[\Phi] + \varepsilon \int_0^L dx \int_0^t dt' \left[m \dot\varphi \dot\eta - ka^2 (\partial_x \varphi)(\partial_x \eta)\right] + \mathcal{O}(\varepsilon^2) =$$

by parts

$$= S[\Phi] + \varepsilon \int_0^L dx \Big[\underbrace{m \dot\varphi\, \eta \Big|_0^t}_{=0} - \int_0^t dt'\, m \ddot\varphi\, \eta \Big] -$$

$$- \varepsilon k a^2 \int_0^t dt' \Big[\underbrace{(\partial_x \varphi)\, \eta \Big|_0^L}_{=0} - \int_0^L dx\, (\partial_x^2 \varphi)\, \eta \Big] + \mathcal{O}(\varepsilon^2)$$

$$\delta S = \lim_{\varepsilon \to 0} \frac{S[\Phi + \eta\varepsilon] - S[\Phi]}{\varepsilon} = -\int_0^t dt' \int_0^L dx \left[m \ddot\Phi - ka^2 (\partial_x^2 \Phi)\right] \eta = 0$$

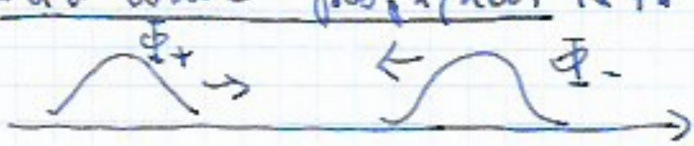
$$\forall \eta$$

$$\Rightarrow \quad \boxed{m \ddot\Phi - k_0 a^2\, \partial_x^2 \Phi = 0} \quad \text{wave equation}$$

$$\left(\frac{\partial}{\partial t} - v \frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + v \frac{\partial}{\partial x}\right) \Phi(x,t) = 0 \qquad v \equiv \sqrt{\frac{k_0 a^2}{m}}$$

$$\Phi(x,t) = \Phi_+(x - vt) + \Phi_-(x + vt)$$

sound wave propagates with $v = \sqrt{\frac{k}{m}}\, a$ to R and L.



Hamiltonian - energy density

$$H = \int_0^L dx \, \mathcal{H} \quad (?)$$

canonically conjugate momenta to $\phi(x,t)$

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = m\dot{\phi} \Rightarrow \dot{\phi} = \frac{1}{m}\pi(x)$$

Legendre transform

$$\mathcal{H}[\phi, \partial_x\phi, \pi] = \pi\dot{\phi} - \mathcal{L}[\phi, \partial_x\phi, \dot{\phi}] =$$

$$\dot{\phi} = \dot{\phi}(\phi, \pi)$$

$$= \frac{\pi^2}{m} - \frac{m}{2}\frac{\pi^2}{m^2} + \frac{k_s a^2}{2}(\partial_x\phi)^2 = \frac{\pi^2}{2m} + \frac{k_s a^2}{2}(\partial_x\phi)^2$$

$$\boxed{\mathcal{H} = \frac{\pi^2}{2m} + \frac{k_s a^2}{2}(\partial_x\phi)^2}$$

Hamiltonian formulation of the classical field theory.

- Poisson brackets in classical mechanics

$$\{A, B\} = \sum_{i=1}^{s}\left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}\right)$$

E.O.M. $\quad \frac{dA}{dt} = \frac{\partial A}{\partial t} - \{\mathcal{H}, A\}$

- in classical field theory

$$\{\phi(x), \pi(x')\} = \int dx''\left(\underbrace{\frac{\delta\phi(x)}{\delta\phi(x'')}}_{\delta(x-x'')}\underbrace{\frac{\delta\pi(x')}{\delta\pi(x'')}}_{\delta(x'-x'')} - \underbrace{\frac{\delta\phi(x)}{\delta\pi(x'')}}_{0}\underbrace{\frac{\delta\pi(x')}{\delta\phi(x'')}}_{0}\right) =$$

$$= \int dx'' \, \delta(x-x')\,\delta(x'-x'') = \delta(x-x')$$

EOM

$$H = \int_0^L dx \left[\frac{\pi^2(x)}{2m} + \frac{k_0 a^2}{2} \left(\partial_x \phi(x)\right)^2 \right]$$

$$\boxed{\dot{\phi}(x)} = \left\{ \phi(x), \int_0^L dy\, \mathcal{H} \right\} =$$

$$= \int dz \int dy \left(\underbrace{\frac{\delta \phi(x)}{\delta \phi(z)}}_{\delta(x-z)} \underbrace{\frac{\delta \mathcal{H}}{\delta \pi(z)}}_{\frac{\pi(y)}{m}\delta(y-z)} - \underbrace{\frac{\delta \phi(x)}{\delta \pi(z)}}_{0} \frac{\delta \mathcal{H}}{\delta \phi(z)} \right) = \boxed{\frac{\pi(x)}{m}}$$

$$\boxed{\dot{\pi}(x)} = \left\{ \pi(x), \int dy\, \mathcal{H} \right\} =$$

$$= \int dz \int dy \left(\underbrace{\frac{\delta \pi(x)}{\delta \phi(z)}}_{0} \frac{\delta \mathcal{H}}{\delta \pi(z)} - \overbrace{\frac{\delta \pi(x)}{\delta \pi(z)}}^{=\delta(x-z)} \frac{\delta \mathcal{H}}{\delta \phi(z)} \right) =$$

$$= -\frac{k_0 a^2}{2} \int dz\, \delta(x-z) \int dy \frac{\delta}{\delta \phi(z)} \left(\partial_y \phi(y)\right)^2 =$$

$$\int dy \frac{\delta}{\delta \phi(x)} (\partial_y \phi(y))(\partial_y \phi(y)) =$$

$$= \int dy \left[\left(\partial_y \frac{\delta \phi(y)}{\delta \phi(x)}\right)(\partial_y \phi(y)) + (\partial_y \phi(y)) \left(\partial_y \frac{\delta \phi(y)}{\delta \phi(x)}\right) \right] =$$

$$= 2 \int dy\, \partial_y \delta(x-y)\, \partial_y \phi(y) =$$

$$= 2\delta(x-y)\, \partial_y \phi(y) \Big|_0^L - 2 \int dy\, \delta(x-y)\, \partial_y^2 \Phi(y)$$

$$= k_0 a^2 \int dz\, \delta(x-z) \int dy\, \delta(y-z)\, \partial_y^2 \Phi(y) = \boxed{k_0 a^2 \partial_x^2 \phi(x)}$$

Eliminating $\dot{\pi}(x)$

$$\ddot{\phi}(x) = \frac{k_0 a^2}{m} \partial_x^2 \phi(x)$$

$$v = \sqrt{\frac{k_0}{m}}\, a$$

$$\boxed{\left(\frac{\partial^2}{\partial t^2} - v^2 \frac{\partial^2}{\partial x^2} \right) \phi(x) = 0}$$

Canonical quantization

→ fields are upgraded to operators

$$\phi(x) \rightarrow \hat{\phi}(x)$$

$$\pi(x) \rightarrow \hat{\pi}(x)$$

→ Poisson brackets are replaced by commutators

$$\{\ ,\ \} \rightarrow [\ ,\ ] \quad \text{with } \delta(x-x') \rightarrow i\hbar\,\delta(x-x')$$

Now, for a chain of atoms / a string

$$\boxed{[\hat{\phi}(x), \hat{\pi}(x')] = i\hbar\,\delta(x-x')}$$

Hamiltonian operator

$$\boxed{\hat{H} = \int dx\ \hat{\mathcal{H}}[\hat{\pi}, \hat{\phi}] = \int dx \left[\frac{\hat{\pi}^2}{2m} + \frac{k_s a^2}{2} (\partial_x \hat{\phi})^2 \right]}$$

To find spectrum $\hat{H}|\psi_\lambda\rangle = E_\lambda |\psi_\lambda\rangle$ and eigenstates we

- make Fourier transform to diagonalize it in k-space
- introduce creation / annihilation operators to factorize the problem

FT

$$\boxed{\begin{aligned} \hat{\phi}_k &= \frac{1}{\sqrt{L}} \int_0^L dx\, e^{-ikx}\, \hat{\phi}(x) \Leftrightarrow \hat{\phi}(x) = \frac{1}{\sqrt{L}} \sum_k e^{ikx}\, \hat{\phi}_k \\ \hat{\pi}_k &= \frac{1}{\sqrt{L}} \int_0^L dx\, e^{+ikx}\, \hat{\pi}(x) \Leftrightarrow \hat{\pi}(x) = \frac{1}{\sqrt{L}} \sum_k e^{-ikx}\, \hat{\pi}_k \end{aligned}}$$

remember $\left.\begin{aligned} \hat{\phi}(x)^+ &= \hat{\phi}(x) \\ \hat{\pi}(x)^+ &= \hat{\pi}(x) \end{aligned}\right\}$ real classical fields

$$\hat{\phi}(x)^+ = \frac{1}{\sqrt{L}} \sum_k e^{-ikx}\, \hat{\phi}_k^+ = \{k \leftrightarrow -k\} = \frac{1}{\sqrt{L}} \sum_k e^{ikx}\, \cancel{e^{ikx}}\, \phi_{-k}^+$$

$$\shortparallel$$

$$\hat{\phi}(x) = \frac{1}{\sqrt{L}} \sum_k e^{ikx}\, \hat{\phi}_k \rightarrow \boxed{\phi_{-k}^+ = \phi_k}$$

Similarly, $\boxed{\pi_{-k}^+ = \pi_k}$

<u>Commutator</u>

$$[\hat{\phi}_k, \hat{\pi}_{k'}] = \frac{1}{L} \int_0^L dx_1 \int_0^L dx_2\, e^{-ikx_1}\, e^{+ik'x_2} \underbrace{[\hat{\phi}(x_1), \hat{\pi}(x_2)]}_{i\hbar\delta(x_1-x_2)} =$$

$$= i\hbar \frac{1}{L} \int_0^L dx_1\, e^{i(k'-k)x_1} = i\hbar\delta_{kk'}$$

$$\boxed{[\hat{\phi}_k, \hat{\pi}_{k'}] = i\hbar\delta_{kk'}}$$

Fourier modes of quantum fields play the same role as components of position and momentum of a simple particle.

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

$$\hat{\vec{x}} = \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \end{pmatrix} \longleftrightarrow \phi(x) = \begin{pmatrix} \hat{\phi}_{k_1} \\ \hat{\phi}_{k_2} \\ \vdots \\ \hat{\phi}_{k_n} \end{pmatrix}$$

Compute

$$\int_0^L dx\,(\partial_x\hat\varphi)^2 = \int dx\left(\partial_x \frac{1}{\sqrt L}\sum_{k_1} e^{ik_1x}\hat\Phi_{k_1}\right)\left(\partial_x \frac{1}{\sqrt L}\sum_{k_2} e^{ik_2x}\hat\Phi_{k_2}\right) =$$

$$= \sum_{k_1 k_2}(-k_1 k_2)\,\hat\Phi_{k_1}\hat\Phi_{k_2}\;\underbrace{\frac{1}{L}\int_0^L dx\, e^{i(k_1+k_2)x}}_{\delta_{k_1,-k_2}} = \sum_k k^2\,\hat\Phi_k\hat\Phi_{-k}$$

$$\int_0^L dx\;\hat\pi^2(x) = \frac{1}{L}\int_0^L dx\left(\sum_{k_1} e^{-ik_1x}\hat\pi_{k_1}\right)\left(\sum_{k_2} e^{-ik_2x}\hat\pi_{k_2}\right) =$$

$$= \sum_{k_1 k_2}\hat\pi_{k_1}\hat\pi_{k_2}\;\underbrace{\frac{1}{L}\int_0^L dx\, e^{-i(k_1+k_2)x}}_{\delta_{k_1,-k_2}} = \sum_k \hat\pi_k\,\hat\pi_{-k}$$

Hence,

$$\boxed{\hat H = \sum_k\left[\frac{1}{2m}\hat\pi_k\hat\pi_{-k} + \frac{k_0 a^2}{2}k^2\,\hat\Phi_k\hat\Phi_{-k}\right]}$$

Df.

$$v = a\sqrt{\frac{k_0}{m}}\,,\qquad \omega_k = v|k|$$

$$\frac{k_0 a^2}{2}k^2 = \frac{m\omega_k^2}{2}$$

$$\boxed{\hat H = \sum_k\left[\frac{1}{2m}\hat\pi_k\hat\pi_{-k} + \frac{m\omega_k}{2}\hat\Phi_k\hat\Phi_{-k}\right]}$$

obvious similarity to harmonic oscillators

$$\left[\begin{aligned}\hat H &= \sum_k \hat H_k\\ \hat H_k &= \frac{1}{2m}\hat\pi_k\hat\pi_{-k} + \frac{m\omega_k}{2}\hat\Phi_k\hat\Phi_{-k}\\ &= \frac{1}{2m}|\hat\pi_k|^2 + \frac{m\omega_k}{2}|\hat\Phi_k|^2\end{aligned}\right]$$

$\hat\pi_k \longleftrightarrow \hat p_k$

$\hat\Phi_k \longleftrightarrow \hat x_k$

$\boxed{\text{Factorization method}}$

Def. Ladder operators for each k

$$\boxed{\begin{aligned}\hat a_k &= \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat\phi_k + \frac{i}{m\omega_k}\hat\pi_k\right)\\ \hat a_k^{\dagger} &= \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat\phi_k - \frac{i}{m\omega_k}\hat\pi_k\right)\end{aligned}}$$

Commutation relations

$$\boxed{[\hat a_k, \hat a_{k'}^{\dagger}]} = \left(\frac{m\omega_k}{2\hbar}\right)\left[\hat\phi_k + \frac{i}{m\omega_k}\hat\pi_k \,,\, \hat\phi_{k'} - \frac{i}{m\omega_k}\hat\pi_{k'}\right] =$$

$$= \left(\frac{m\omega_k}{2\hbar}\right)\left(-\frac{i}{m\omega_k}\underbrace{[\hat\phi_k, \hat\pi_{k'}]}_{=\, i\hbar\delta_{kk'}} + \frac{i}{m\omega_k}\underbrace{[\hat\pi_k, \hat\phi_{k'}]}_{=\, -i\hbar\delta_{kk'}}\right) =$$

$$= \left(\frac{\cancel{m\omega_k}}{2\hbar}\right)\left(-\frac{i}{\cancel{m\omega_k}}\right)\left(\underbrace{i\hbar\delta_{kk'} + i\hbar\delta_{kk'}}_{2i\hbar\delta_{kk'}}\right) = \boxed{\delta_{kk'}}$$

$$[\hat a_k, \hat a_{k'}] = [\hat a_k^{\dagger}, \hat a_k^{\dagger}] = 0.$$

Hamiltonian in factorized form

$$\boxed{\begin{aligned}\hat\phi_k &= \sqrt{\frac{\hbar}{2m\omega_k}}\left(\hat a_k + \hat a_{-k}^{\dagger}\right)\\ \hat\pi_k &= i\sqrt{\frac{\hbar m\omega_k}{2}}\left(\hat a_k^{\dagger} - \hat a_{-k}\right)\end{aligned}}$$

$$\sum_k \frac{1}{2m}\hat\pi_k\hat\pi_{-k} = \sum_k \frac{1}{2m}\left(-\frac{\hbar m\omega_k}{2}\right)\left(\hat a_k^\dagger - \hat a_{-k}\right)\left(\hat a_{-k}^\dagger - \hat a_k\right)$$

$$= -\frac{1}{4}\sum_k \hbar\omega_k\left(\underline{\hat a_k^\dagger \hat a_{-k}^\dagger} - \hat a_k^\dagger\hat a_k - \hat a_{-k}\hat a_{-k}^\dagger + \hat a_{-k}\hat a_k\right)$$

$$\sum_k \frac{m\omega_k^2}{2}\hat\phi_k\hat\phi_{-k} = \sum_k\frac{m\omega_k^2}{2}\left(\frac{\hbar}{2m\omega_k}\right)\left(\hat a_k + \hat a_{-k}^\dagger\right)\left(\hat a_{-k}+\hat a_k^\dagger\right)=$$

$$=\frac{1}{4}\sum_k\hbar\omega_k\left(\hat a_k\hat a_{-k} + \hat a_k\hat a_k^\dagger + \hat a_{-k}^\dagger \hat a_{-k} + \underline{\hat a_{-k}^\dagger\hat a_k^\dagger}\right)$$

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

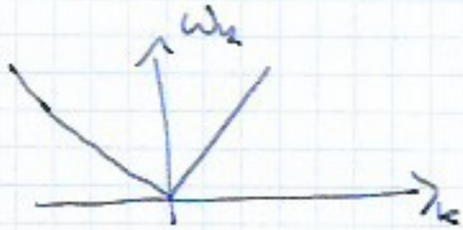
$$\hat H=\sum_k\hat H_k\,,\qquad \hat H_k=\hbar\omega_k\left(\hat a_k^\dagger\hat a_k+\tfrac{1}{2}\right)$$

$$\hat H|E\rangle = E|E\rangle \qquad \hat H_k|n_k\rangle=\hbar\omega_k\left(n_k+\tfrac{1}{2}\right)|n_k\rangle$$

$$E=\sum_k\hbar\omega_k\left(n_k+\tfrac{1}{2}\right) \qquad |n_k\rangle = \frac{(\hat a_k^\dagger)^{n_k}}{\sqrt{n_k!}}|v\rangle$$

$$|E\rangle = \bigotimes_k |n_k\rangle$$

$$\omega_k = v|k|$$



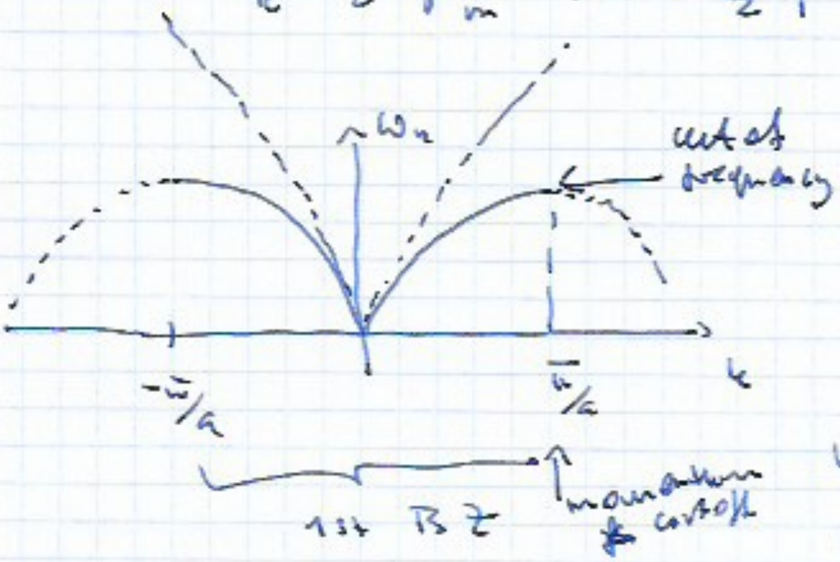
$$\omega_k \xrightarrow[k\to 0]{} 0 \qquad \text{Goldstone mode}$$

$\boxed{\hat a_k^\dagger}$ - creates a quasiparticle - phonon

Counting number of states

- discrete case (lecture)

$$\omega_k = 2\sqrt{\frac{k_0}{m}}\left|\sin\frac{ka}{2}\right| \qquad + \text{P.B.C.}$$



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

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

$$\omega^{cut} = 2\sqrt{\frac{k_0}{m}}$$

$$k^{cut} = \pi/a$$

$$\omega_k \underset{k\to 0}{\to} \left(\sqrt{\frac{k_0}{m}}\, a\right) k = v k$$

Waves with $\lambda < a$ are not allowed in a chain of atoms. They are allowed in a continuum system.