Discrete: Classical Mechanics of Point Particles - Monatomic Chain

$$M\ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n) \Leftarrow \text{Newton's law}$$

- we apply periodic B.C. $\Rightarrow$ q discretized
- Monatomic chain with N atoms (N unit cells)

$$u_n(t) = \underset{\uparrow}{\frac{1}{\sqrt{N}}} e^{iqna} \underbrace{e^{-i\omega(q)t} A_q}_{B_q(t)} = \frac{1}{\sqrt{N}} e^{iqna} B_q(t)$$

just a normalization factor

where $q \in 1^{st}$ B.Z.

- Substitute into eqs. of motion gives

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

dispersion relation

- note: $\omega(-q) = \omega(q)$

- General solution takes on the form:

$$\underset{\substack{\uparrow \\ \text{real}}}{u_n(t)} = \sum_q \left(\frac{1}{\sqrt{N}} e^{iqna} e^{-i\omega(q)t} A_q + \underbrace{\frac{1}{\sqrt{N}} e^{-iqna} e^{i\omega(q)t} A_q^*}_{\text{c.c.}} \right)$$

At $t=0$, if $u_n(0)$ and $\dot{u}_n(0)$ are given, then A_q and A_q^* are fixed. Subsequently, at time t, solution is given by $u_n(t)$.

Note that one can also write:

$$u_n(t) = \sum_q \frac{1}{\sqrt{N}} e^{iqna} e^{-i\omega(q)t} A_q + \sum_q \frac{1}{\sqrt{N}} e^{-iqna} e^{i\omega(q)t} A_q^*$$

$$= \sum_q \frac{1}{\sqrt{N}} e^{iqna} e^{-i\omega(q)t} A_q + \sum_{q'} \frac{1}{\sqrt{N}} e^{iq'na} e^{i\omega(-q')t} A_{-q'}^*$$

$$= \sum_q \frac{1}{\sqrt{N}} e^{iqna} e^{-i\omega(q)t} A_q + \sum_q \frac{1}{\sqrt{N}} e^{iqna} e^{i\omega(q)t} A_{-q}^*$$

$$= \sum_q \frac{1}{\sqrt{N}} e^{iqna} \left(e^{-i\omega(q)t} A_q + e^{i\omega(-q)t} A_{-q}^* \right)$$

$$= \sum_q \frac{1}{\sqrt{N}} e^{iqna} \left(B_q + B_{-q}^* \right)$$

← sometimes this form is more convenient.

Note that quite generally, $\omega(-q) = \omega(q)$.

Lagrangian and Hamiltonian

$$T = \sum_{n=1}^{N} \frac{1}{2} M \dot{u}_n^2 \quad ; \quad V = \frac{1}{2} K \sum_{n=1}^{N} (u_n - u_{n+1})^2$$

- Lagrangian equations:

$$\left. \begin{array}{l} L = T - V \\ \dfrac{d}{dt} \dfrac{\partial L}{\partial \dot{u}_n} - \dfrac{\partial L}{\partial u_n} = 0 \end{array} \right\} \text{give equations of motion}$$

- Define conjugate momentum $p_n = \dfrac{\partial L}{\partial \dot{u}_n}$

$$p_n = M \dot{u}_n$$

- Define $H = \sum_n p_n \dot{u}_n - L$

$$H = \sum_n \frac{p_n^2}{2M} + \frac{K}{2} \sum_n (u_n - u_{n+1})^2$$

- Hamilton equations $\dot{u}_n = \dfrac{\partial H}{\partial p_n}$; $\dot{p}_n = -\dfrac{\partial H}{\partial u_n}$

For monatomic chain,

$$\dot{u}_n = \frac{p_n}{M} \quad ; \quad \dot{p}_n = K(u_{n+1} + u_{n-1} - 2u_n)$$

(same as before)

<u>Task:</u> Write $H = \sum_n \frac{p_n^2}{2M} + \frac{K}{2}\sum_n (u_n - u_{n+1})^2 = K.E. + P.E.$
in terms of A_q, A_q^* (OR B_q, B_q^*).

$$p_n = M\dot{u}_n = \sum_q \left(-i\omega(q)M\frac{1}{\sqrt{N}}e^{iqna}e^{-i\omega(q)t}A_q + i\omega(q)M\frac{1}{\sqrt{N}}e^{-iqna}e^{i\omega(q)t}A_q^*\right)$$

$$= \sum_q \left(-i\omega(q)M\frac{1}{\sqrt{N}}e^{iqna}B_q(t) + c.c.\right)$$

<u>k.e. term:</u>

$$\frac{1}{2M}\sum_n p_n^2 = \frac{1}{2M}\sum_n\left(\sum_q\left(-i\omega(q)\frac{M}{\sqrt{N}}e^{iqna}B_q(t) + c.c.\right)\right)^2$$

$$= \frac{1}{2M}\sum_n\sum_q\sum_{q'}\left(-i\omega(q)\frac{M}{\sqrt{N}}e^{iqna}B_q + i\omega(q)\frac{M}{\sqrt{N}}e^{-iqna}B_q^*\right)\cdot$$
$$\left(-i\omega(q')\frac{M}{\sqrt{N}}e^{iq'na}B_{q'} + i\omega(q')\frac{M}{\sqrt{N}}e^{-iq'na}B_{q'}^*\right)$$

$$= (1) + (2) + (3) + (4) \qquad (4 \text{ terms})$$

$$(1) = \frac{1}{2M}\sum_q\sum_{q'} -\omega(q)\omega(q')M^2 B_q B_{q'} \underbrace{\frac{1}{N}\sum_n e^{i(q+q')na}}_{\delta_{q',-q}}$$

$$= \frac{M}{2}\sum_q -\omega(q)\omega(-q)B_q B_{-q}$$

Note:
$q, q' \in 1^{st}$ B.Z.
- only when $q+q'=0$, $\sum_n 1 = N$
- Otherwise, 0.

$$(2) = \frac{1}{2M}\sum_q\sum_{q'} -\omega(q)\omega(q')M^2 B_q^* B_{q'}^* \underbrace{\frac{1}{N}\sum_n e^{-i(q+q')na}}_{\delta_{q',-q}}$$

$$= \frac{M}{2}\sum_q -\omega(q)\omega(-q)B_q^* B_{-q}^*$$

$$3 = \frac{1}{2M}\sum_q \sum_{q'} \omega(q)\omega(q') M^2 B_q B^*_{q'} \underbrace{\frac{1}{N}\sum_n e^{i(q-q')na}}_{\delta_{q,q'}}$$

$$= \frac{M}{2}\sum_q \omega(q)\omega(q) B_q B^*_q = \frac{M}{2}\sum_q \omega^2(q) B_q B^*_q$$

$$4 = \frac{1}{2M}\sum_q \sum_{q'} \omega(q)\omega(q') M^2 B^*_q B_{q'} \underbrace{\frac{1}{N}\sum_n e^{-i(q-q')na}}_{\delta_{q,q'}}$$

$$= \frac{M}{2}\sum_q \omega^2(q) B^*_q B_q$$

Thus, the k.e. term is:

$$\frac{1}{2M}\sum_n P_n^2 = \frac{M}{2}\sum_q \Big(-\omega(q)\omega(-q) B_q(t) B_{-q}(t) - \omega(q)\omega(-q) B^*_q(t) B^*_{-q}(t)$$
$$+ \omega^2(q) B_q(t) B^*_q(t) + \omega^2(q) B^*_q(t) B_q(t)\Big)$$

* Note: order of B, B^* has been intentionally kept.

p.e. term:

$$V = \frac{K}{2}\sum_n (u_n - u_{n+1})^2 = \frac{K}{2}\sum_n \left(u_n^2 + u_{n+1}^2 - 2u_n u_{n+1}\right)$$

$$= \underbrace{K\sum_n u_n^2}_{a} \underbrace{- \frac{K}{2}\sum_n u_{n-1}u_n}_{b} \underbrace{- \frac{K}{2}\sum_n u_{n+1}u_n}_{c}$$

actually the same!

$$(a) = K\sum_q \sum_{q'} \sum_n \Big(\frac{1}{\sqrt{N}} e^{iqna} \overbrace{e^{-i\omega(q)t} A_q}^{B_q} + \frac{1}{\sqrt{N}} e^{-iqna} \overbrace{e^{i\omega(q)t} A_q^*}^{B_q^*}\Big)\Big(\frac{1}{\sqrt{N}} e^{iq'na} \overbrace{e^{-i\omega(q')t} A_{q'}}^{B_{q'}} + \frac{1}{\sqrt{N}} e^{-iq'na} \overbrace{e^{i\omega(q')t} A_{q'}^*}^{B_{q'}^*}\Big)$$

$$= K\sum_q \Big(B_q(t) B_{-q}(t) + B_q^*(t) B_{-q}^*(t) + B_q(t) B_q^*(t) + B_q^*(t) B_q(t)\Big)$$

$$(b) = \frac{K}{2}\sum_n \sum_q \sum_{q'} \Big(\frac{1}{\sqrt{N}} e^{iq(n-1)a} B_q + \frac{1}{\sqrt{N}} e^{-iq(n-1)a} B_q^*\Big)\Big(\frac{1}{\sqrt{N}} e^{iq'na} B_{q'} + \frac{1}{\sqrt{N}} e^{-iq'na} B_{q'}^*\Big)$$

$$= \frac{K}{2}\sum_q \Big(B_q(t) B_{-q}(t) e^{-iqa} + B_q^*(t) B_{-q}^*(t) e^{iqa} + B_q(t) B_q^*(t) e^{-iqa} + B_q^*(t) B_q(t) e^{iqa}\Big)$$

$$(c) = \frac{K}{2}\sum_n \sum_q \sum_{q'} \Big(\frac{1}{\sqrt{N}} e^{iq(n+1)a} B_q + \frac{1}{\sqrt{N}} e^{-iq(n+1)a} B_q^*\Big)\Big(\frac{1}{\sqrt{N}} e^{iq'na} B_{q'} + \frac{1}{\sqrt{N}} e^{-iq'na} B_{q'}^*\Big)$$

$$= \frac{K}{2}\sum_q \Big(B_q(t) B_{-q}(t) e^{iqa} + B_q^*(t) B_{-q}^*(t) e^{-iqa} + B_q(t) B_q^*(t) e^{iqa} + B_q^*(t) B_q(t) e^{-iqa}\Big)$$

$H = T + V$

$\omega(q)\omega(-q) = \omega(q)^2$

$B_q(t) B_{-q}(t)$ terms: $\sum_q \underbrace{\Big(-\omega^2(q)\frac{M}{2} + K - \frac{K}{2} e^{-iqa} - \frac{K}{2} e^{iqa}\Big)}_{=0} B_q(t) B_{-q}(t) = 0$

because $-\omega^2(q) = \frac{2K}{M}(\cos qa - 1)$ is the dispersion relation

$B_q^*(t) B_{-q}^*(t)$ terms: $\sum_q \underbrace{\Big(-\omega^2(q)\frac{M}{2} + K - \frac{K}{2} e^{iqa} - \frac{K}{2} e^{-iqa}\Big)}_{=0} B_q^*(t) B_{-q}^*(t) = 0$

same reason

Thus, only terms $\sim B_q B_q^*$ and $\sim B_q^* B_q$ in H.

$B_q^*(t)\,B_q(t)$ terms: $\sum_q \Big(\omega^2(q)\frac{M}{2} + \underbrace{K - \frac{K}{2}e^{iqa} - \frac{K}{2}e^{-iqa}}_{\omega^2(q)\frac{M}{2}}\Big) B_q^*(t)\,B_q(t)$

$$= \sum_q M\omega^2(q)\, B_q^*(t)\, B_q(t)$$

$B_q(t)\,B_q^*(t)$ terms: $\sum_q \Big(\omega^2(q)\frac{M}{2} + \underbrace{K - \frac{K}{2}e^{-iqa} - \frac{K}{2}e^{iqa}}_{\omega^2(q)\frac{M}{2}}\Big) B_q(t)\,B_q^*(t)$

$$= \sum_q M\omega^2(q)\, B_q(t)\, B_q^*(t)$$

Therefore, the total Hamiltonian is given by:

$$\boxed{H = \sum_q M\omega^2(q)\left[B_q^*(t)\,B_q(t) + B_q(t)\,B_q^*(t)\right]}$$

This is the end of the classical mechanical treatment.

- For later purpose, one may introduce $\hbar$ into H:

$$H = \sum_q \frac{\hbar\omega(q)}{2}\,\frac{2M\omega(q)}{\hbar}\left(B_q^*(t)\,B_q(t) + B_q(t)\,B_q^*(t)\right)$$

$$= \sum_q \frac{\hbar\omega(q)}{2}\left(b_q^*(t)\,b_q(t) + b_q(t)\,b_q^*(t)\right)$$

where $B_q(t) \equiv \sqrt{\frac{\hbar}{2M\omega(q)}}\; b_q(t)$.

But note that up to here, there is nothing quantum mechanical!
($\hbar$ is introduced simply as a constant)

Discrete: Quantum Mechanics – Monatomic Chain

- From L, define p_n corresponding to u_n
- Classical Mechanics → Quantum Mechanics $\begin{array}{l} u_\ell \to \hat{u}_\ell \\ p_\ell \to \hat{p}_\ell \end{array}$

Impose: $\begin{cases} p_n u_\ell - u_\ell p_n = -i\hbar\,\delta_{n\ell} \text{ OR } [p_n, u_\ell] = -i\hbar\,\delta_{n\ell} \\ [u_n, u_\ell] = 0 \; ; \; [p_n, p_\ell] = 0 \end{cases}$ "^" omitted

Aim: Explore the commutation relation between B_q, $B^*_{q'}$

Recall:

$$u_n(t) = \sum_q \frac{1}{\sqrt{N}} e^{iqna}\left(B_q(t) + B^*_{-q}(t)\right)$$

Thus, $(B_q + B^*_{-q})$ is the Fourier coefficient of $u_n(t)$

$$\underbrace{B_q(t) + B^*_{-q}(t)}_{\equiv \alpha_q(t)} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-iqna} u_n(t) \equiv \alpha_q(t)$$

$$p_n(t) = M\dot{u}_n(t) = \sum_q -i\omega(q)\frac{M}{\sqrt{N}} e^{iqna} B_q(t) + i\omega(q)\frac{M}{\sqrt{N}} e^{+iqna} B^*_{-q}(t)$$

$$= \sum_q \frac{1}{\sqrt{N}} e^{iqna}\left(-i\omega(q) M B_q(t) + i\omega(-q) M B^*_{-q}(t)\right)$$

$$\therefore \underbrace{\left(-i B_q(t) + i B^*_{-q}(t)\right)}_{\beta_q(t)} M\omega(q) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-iqna} p_n(t)$$

$$\beta_q(t)\, M\omega(q) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-iqna} p_n(t)$$

Thus,
$$\begin{cases} \alpha_q = B_q + B^*_{-q} \\ \beta_q = -i B_q + i B^*_{-q} \end{cases}$$

OR
$$B_q(t) = \frac{1}{2}\left(\alpha_q(t) + i\beta_q(t)\right)$$
$$B^*_{-q}(t) = \frac{1}{2}\left(\alpha_q(t) - i\beta_q(t)\right)$$

In full form,
$$B_q(t) = \left(\frac{1}{2}\sum_n \frac{1}{\sqrt{N}} e^{-iqna} u_n(t) + \frac{i}{2}\sum_n \frac{1}{\sqrt{N}} e^{-iqna} \frac{p_n(t)}{M\omega(q)}\right)$$
$$= \sum_n \left(\frac{1}{2\sqrt{N}} u_n(t) + \frac{i}{2\sqrt{N}} \frac{1}{M\omega(q)} p_n(t)\right) e^{-iqna}$$
$$B^*_{-q}(t) = \sum_n \left(\frac{1}{2\sqrt{N}} u_n(t) - \frac{i}{2\sqrt{N}} \frac{1}{M\omega(q)} p_n(t)\right) e^{-iqna}$$

OR
$$B^*_q(t) = \sum_n \left(\frac{1}{2\sqrt{N}} u_n(t) - \frac{i}{2\sqrt{N}} \frac{1}{M\omega(q)} p_n(t)\right) e^{iqna}$$

Thus, B_q, B^*_q are expressed in terms of u_n, p_ℓ.

Commutators of $[u_n, p_\ell]$, etc. $\Rightarrow$ Commutators of $[B_q, B^*_{q'}]$ etc.

$[B_q, B^*_{q'}] = ?$ $\qquad$ $B_q(t)$ and $B_{q'}(t)$ same time t

$$[B_q, B^*_{q'}] = \frac{1}{4}\Big((\alpha_q + i\beta_q)(\alpha_{-q'} - i\beta_{-q'}) - (\alpha_{-q'} - i\beta_{-q'})(\alpha_q + i\beta_q)\Big)$$

$$= \frac{1}{4}\Big([\alpha_q, \alpha_{-q'}] + [\beta_q, \beta_{-q'}] + i[\beta_q, \alpha_{-q'}] - i[\alpha_q, \beta_{-q'}]\Big)$$

Recall: $\alpha_q = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{-iqna} u_n(t)$; $\beta_q = \frac{1}{M\omega(q)}\frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{-iqna} p_n(t)$

$\therefore$ $[\alpha_q, \alpha_{-q'}] \sim [u_n, u_{n'}] = 0$; $[\beta_q, \beta_{-q'}] \sim [p_n, p_{n'}] = 0$

Thus, $[B_q, B^*_{q'}] = \frac{i}{4}\Big([\beta_q, \alpha_{-q'}] - [\alpha_q, \beta_{-q'}]\Big)$

$$= \frac{i}{4}\Big([\beta_q, \alpha_{-q'}] + [\beta_{-q'}, \alpha_q]\Big)$$

$$[\beta_q, \alpha_{-q'}] = \frac{1}{N}\frac{1}{M\omega(q)}\sum_n e^{-iqna}\sum_{n'} e^{iq'n'a}[p_n, u_{n'}]$$

$$= \frac{1}{N}\frac{1}{M\omega(q)}\sum_n e^{-iqna}\sum_{n'} e^{iq'n'a}\,\frac{\hbar}{i}\delta_{nn'}$$

$$= \frac{1}{N}\frac{1}{M\omega(q)}\sum_n e^{ina(q'-q)}\frac{\hbar}{i} = \frac{\hbar}{i}\frac{1}{M\omega(q)}\delta_{q,q'}$$

$$[\beta_{-q'}, \alpha_q] = \frac{\hbar}{i}\frac{1}{M\omega(-q)}\delta_{q,q'} = \frac{\hbar}{i}\frac{1}{M\omega(q)}\delta_{q,q'}$$

$\therefore$ $[B_q, B^*_{q'}] = \frac{i}{4}\frac{\hbar}{i}\cdot\frac{1}{M\omega(q)}\delta_{q,q'}\cdot 2 = \frac{\hbar}{2M\omega(q)}\delta_{q,q'}$

which is the required commutator.

$$\Big[\underbrace{\sqrt{\frac{2M\omega(q)}{\hbar}}\, B_q}\ ,\ \sqrt{\frac{2M\omega(q')}{\hbar}}\, B_{q'}^{*}\Big] = \delta_{q,q'}$$

$$[\,b_q\ ,\ b_{q'}^{*}\,] = \delta_{q,q'}\ ,\quad \text{usually written as } [b_q, b_{q'}^{+}] = 0$$

Similarly, one can find $[B_q, B_{q'}]$, $[B_q^*, B_{q'}^*]$

The result is $[b_q, b_{q'}] = 0$, $[b_q^*, b_{q'}^*] = 0$ or $[b_q^+, b_{q'}^+] = 0$

$$\therefore\ \hat{H} = \sum_q \frac{\hbar\omega(q)}{2}\left[\,b_q^{+} b_q + b_q b_q^{+}\right]$$

$$= \sum_q \frac{\hbar\omega(q)}{2}\left[\,b_q^{+} b_q + 1 + b_q^{+} b_q\right]$$

$$= \sum_q \frac{\hbar\omega(q)}{2} + \sum_q \hbar\omega(q)\, b_q^{+} b_q$$

which is just a collection of quantum oscillators.

- In short, one starts with

$$\hat{H} = \sum_{n=1}^{N} \frac{\hat{p}_n^2}{2M} + \frac{1}{2}\sum_n (\hat{u}_n - \hat{u}_{n+1})^2$$

with $[\hat{p}_n, \hat{u}_\ell] = \frac{\hbar}{i}\delta_{n\ell}$, etc.

Introduce: b_q, b_q^+ through

$$\begin{cases} u_n(t) = \sum_q \sqrt{\frac{\hbar}{2M\omega(q)N}}\,(b_q(t) + b_{-q}^+(t))\, e^{iqna} \\ p_n(t) = -i\sum_q \sqrt{\frac{\hbar M\omega(q)}{2N}}\,(b_q(t) - b_{-q}^+(t))\, e^{iqna} \end{cases}$$

OR

$$\begin{cases} b_q(t) = \sum_n \left(\sqrt{\frac{M\omega(q)}{2\hbar N}}\, u_n(t) + i\sqrt{\frac{1}{2\hbar M\omega(q)N}}\, p_n(t)\right) e^{-iqna} \\ b_q^+(t) = \sum_n \left(\sqrt{\frac{M\omega(q)}{2\hbar N}}\, u_n(t) - i\sqrt{\frac{1}{2\hbar M\omega(q)N}}\, p_n(t)\right) e^{iqna} \end{cases}$$

and then $\hat{H}$ becomes

$$\boxed{\hat{H} = \sum_q \frac{\hbar\omega(q)}{2} + \sum_q \hbar\omega(q)\, b_q^+ b_q}$$

Schrödinger Equation is:

$$\left(\sum_q \hbar\omega(q)\, b_q^+ b_q\right)\Psi = E\Psi$$

Eigenstate is characterized by $|\{n_q\}\rangle$

occupation numbers
(# phonons)

In this form, the formalism can treat system with different numbers of (quasi-) particles.

From chain to string

Continuum: Classical Field Theory

1. An equation for the field

- For the string problem, we have the discrete chain as a guide. In other problems, we can identify the equation from either classical physics or quantum physics. In some problems, one simply constructs a Lagrangian using reasonable arguments.
- For the chain, consider

$N \to \infty$, $a \to 0$, such that $Na = L =$ finite

↳ (from discrete to continuum)

Discrete: label n Continuum: $na = x$

(x is a continuous variable)

Discrete equation of motion:

$$M\ddot{u}_n(t) = K(u_{n+1} + u_{n-1} - 2u_n)$$

Task: turn eq. into continuous version

$\Delta n = 1 , \quad x = na , \quad \Delta x = \Delta n \cdot a$

Writing $\frac{M}{a} = \rho$ (mass density)

OR $M = \rho a$

$$\rho a \, \ddot{u}_x(t) = Ka \frac{\left[u_{x+\Delta x}(t) + u_{x-\Delta x}(t) - 2u_x(t)\right]}{a}$$

$$= Ka \left[\frac{u_{x+\Delta x}(t) - u_x(t)}{\Delta x} - \frac{u_x(t) - u_{x-\Delta x}(t)}{\Delta x}\right]$$

$$= Ka^2 \frac{1}{\Delta x}\left[\frac{u_{x+\Delta x}(t) - u_x(t)}{\Delta x} - \frac{u_x(t) - u_{x-\Delta x}(t)}{\Delta x}\right]$$

$$= Ka^2 \frac{1}{\Delta x}\left[\left.\frac{\partial u(x,t)}{\partial x}\right|_{x+\frac{\Delta x}{2}} - \left.\frac{\partial u(x,t)}{\partial x}\right|_{x-\frac{\Delta x}{2}}\right]$$

$$= Ka^2 \frac{\partial^2 u(x,t)}{\partial x^2}$$

$$\Rightarrow \boxed{\rho \ddot{u}(x,t) = Ka \frac{\partial^2 u(x,t)}{\partial x^2}} = g \frac{\partial^2 u(x,t)}{\partial x^2}$$

- standard wave equation
- $a \to 0$, $Ka \to$ finite $= g$
- Continuum: $a \to 0$, always in long wavelength limit, i.e., picks up low-energy excitations
- $u(x,t)$ is the field (displacement field) in the problem. It gives the displacement from equilibrium at x at time t.

$$\boxed{\rho \frac{\partial^2 u(x,t)}{\partial t^2} = g \frac{\partial^2 u(x,t)}{\partial x^2} \quad \text{is the field equation}}$$

* Proceed to look for the dispersion relation

$$u(x,t) = \frac{1}{\sqrt{L}} e^{iqx} e^{-i\omega(q)t} A_q = \frac{1}{\sqrt{L}} e^{iqx} B_q(t)$$

Substitute into field equation:

$$-\omega^2(q) \rho B_q(t) = -g\, q^2 B_q(t)$$

$$\Rightarrow \boxed{\omega^2(q) = \frac{g}{\rho} q^2 \quad \text{i.e. } \omega \sim q}$$

dispersion relation — as expected for long wavelength excitations

Continuum: No atomic scale periodicity any more^{+}

Periodic B.C.:

$$u(x+L,t) = u(x,t)$$

$$\Rightarrow q = \frac{2\pi}{L} \cdot n; \quad n = 0, \pm 1, \pm 2, \cdots \text{ (no restriction)}$$

Properties:

$$\left.\begin{aligned} &\int_0^L \left(\frac{1}{\sqrt{L}} e^{iqx}\right)^* \left(\frac{1}{\sqrt{L}} e^{iqx}\right) dx = 1 \\ &\int_0^L \left(\frac{1}{\sqrt{L}} e^{iqx}\right)^* \left(\frac{1}{\sqrt{L}} e^{iq'x}\right) dx = 0, \quad q \neq q' \end{aligned}\right\} \text{orthonormal property}$$

$^{+}$Don't need to restrict q to 1st B.Z.

<u>Task</u>: Construct a Lagrangian L when plugged into a <u>continuum form of the Lagrangian equation</u> gives the field equation.

<u>Why?</u> If you can do this, we can define the conjugate momentum, Hamiltonian, and get prepared for imposing commutation relations.

Again, guided by discrete equations.

$$L = T - V$$

$$T = \sum_n \frac{1}{2} M \dot{u}_n^2 \quad \text{(discrete)}$$

$$= \sum_n \frac{1}{2} \rho a \dot{u}_n^2$$

$$a \to \Delta x \qquad \dot{u}_n^2 \to \left(\frac{\partial u(x,t)}{\partial t}\right)^2$$

$$\boxed{T = \int_0^L \frac{1}{2} \rho (\dot{u}(x,t))^2} \leftarrow \text{continuum}$$

Note: T is a function of a function! (functional)

$$V = \frac{K}{2}\sum_n (u_n - u_{n+1})^2$$

$$= \frac{1}{2}\sum_n \underbrace{(Ka)}_{g} \frac{\overset{\swarrow \Delta x}{a}}{\underset{\nwarrow (\Delta x)^2}{a^2}} (u_n - u_{n+1})^2$$

$$V = \frac{1}{2}\int_0^L g\left(\frac{\partial u(x,t)}{\partial x}\right)^2 dx$$

$$\therefore \boxed{\begin{aligned} L &= \int_0^L \frac{1}{2}\rho\left(\frac{\partial u(x,t)}{\partial t}\right)^2 dx - \int_0^L \frac{1}{2} g\left(\frac{\partial u(x,t)}{\partial x}\right)^2 dx \\ &= \int_0^L \underset{\uparrow \text{ Lagrangian density}}{\mathcal{L}}\, dx \qquad \text{Note: } L = L(t) \end{aligned}}$$

- $L\left[u(x,t), \frac{\partial u(x,t)}{\partial x}, \frac{\partial u(x,t)}{\partial t}\right]$ OR $L[u(x,t), \dot{u}(x,t)]^{+}$
- $\mathcal{L}\left(u(x,t), \frac{\partial u(x,t)}{\partial x}, \dot{u}(x,t)\right)$ is useful in local field theory.
- In field theory notations, the field is usually written as $\phi(x,t)$ instead of $u(x,t)$.

+ Note: $L(t)$. $L[u(x,t), \dot{u}(x,t)]$ is analogous to $L[q,\dot{q}]$, i.e., depends on u and $\dot{u}$ at <u>all points</u> x in space, but $L(t)$ doesn't depend on x itself.

What is the appropriate Lagrangian Equation?

Motivated by what was done in discrete case.

$$L = T - V = \sum_n \frac{M}{2} \dot{u}_n^2 - \sum_n \frac{K}{2} (u_n - u_{n+1})^2$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{u}_n}\right) - \frac{\partial L}{\partial u_n} = 0$$

$$\frac{\partial L}{\partial \dot{u}_n} = \frac{\partial}{\partial \dot{u}_n} \sum_{n'} \frac{M}{2} \dot{u}_{n'}^2 = \sum_{n'} \frac{M}{2} 2\dot{u}_{n'} \underbrace{\frac{\partial \dot{u}_{n'}}{\partial \dot{u}_n}}_{\delta_{nn'}} = M\dot{u}_n$$

$$\frac{\partial L}{\partial u_n} = -\frac{K}{2} \frac{\partial}{\partial u_n} \sum_{n'} (u_{n'} - u_{n'+1})^2$$

$$= -K \sum_{n'} (u_{n'} - u_{n'+1}) \left(\underbrace{\frac{\partial u_{n'}}{\partial u_n}}_{\delta_{nn'}} - \underbrace{\frac{\partial u_{n'+1}}{\partial u_n}}_{\delta_{n,n'+1}} \right)$$

$$= -K(u_n - u_{n+1}) + K(u_{n-1} - u_n)$$

$$= K(u_{n+1} + u_{n-1} - 2u_n)$$

$$\therefore M\ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n) \text{ as expected}$$

Note that in the steps, we used

$$\frac{\partial \dot{u}_{n'}}{\partial \dot{u}_n} = \delta_{nn'} \; ; \quad \frac{\partial u_{n'}}{\partial u_n} = \delta_{nn'}$$

Now, $u_n(t) \rightarrow u(x,t)$

We need to consider derivatives like $\dfrac{\partial \dot{u}(x)}{\partial \dot{u}(x')}$?!

Define derivatives: new kind of derivatives

$$\frac{\delta u(x)}{\delta u(x')} = \delta(x-x')$$

Dirac δ-function

$$\int_{x_1}^{x_2} f(x)\,\delta(x-a)\,dx = f(a) \qquad x_1 < a < x_2$$

$$\frac{\delta \dot{u}(x)}{\delta \dot{u}(x')} = \delta(x-x')$$

Chain rule still applies

$$\frac{\delta f(u(x))}{\delta u(x')} = \frac{\partial f(u(x))}{\partial u(x)}\,\frac{\delta u(x)}{\delta u(x')}$$

Recall: $L = \int_0^L \frac{1}{2}\rho\,\dot{u}(x)^2\,dx - \int_0^L \frac{1}{2} g \left(\frac{\partial u(x)}{\partial x}\right)^2 dx$

We want to see if

$$\frac{d}{dt}\frac{\delta L}{\delta \dot{u}(x)} - \frac{\delta L}{\delta u(x)} = 0$$

a natural extension of the equation in the discrete case

would give

$$\rho\,\frac{\partial^2 u}{\partial t^2} = g\,\frac{\partial^2 u}{\partial x^2}$$

$$\frac{\delta L}{\delta \dot{u}(x)} = \frac{\delta}{\delta \dot{u}(x)} \left(\int_0^L \frac{1}{2} \rho \, \dot{u}(x')^2 \, dx' \right)$$

$$= \frac{1}{2} \int_0^L \rho \, \frac{\delta \, \dot{u}(x')^2}{\delta \dot{u}(x)} \, dx'$$

$$= \frac{1}{2} \int_0^L \rho \, 2 \, \dot{u}(x') \, \frac{\delta \dot{u}(x')}{\delta \dot{u}(x)} \, dx' \qquad \text{chain rule}$$

$$= \int_0^L \rho \, \dot{u}(x') \, \delta(x'-x) \, dx'$$

$$= \rho \dot{u}(x)$$

$$\frac{d}{dt} \frac{\delta L}{\delta \dot{u}(x)} = \rho \ddot{u}(x)$$

which is the time-derivative term in the wave (field) equation

$\therefore$ looks promising!

$$\frac{\delta L}{\delta u(x)} = \int_0^L -\frac{1}{2} g \, \frac{\delta}{\delta u(x)} \left(\frac{\partial u(x')}{\partial x'} \right)^2 dx'$$

$$= -\int_0^L g \, \frac{\partial u(x')}{\partial x'} \underbrace{\frac{\delta}{\delta u(x)} \left(\frac{\partial u(x')}{\partial x'} \right)}_{\text{what is this?}} dx'$$

Let's work it out

$$\boxed{\begin{aligned}
\frac{\partial u(x')}{\partial x'} &= \frac{u(x'+dx') - u(x')}{dx'} \qquad (dx' \to 0)\\
\frac{\delta}{\delta u(x)}\left(\frac{\partial u(x')}{\partial x'}\right) &= \frac{1}{dx'}\left[\frac{\delta u(x'+dx')}{\delta u(x)} - \frac{\delta u(x')}{\delta u(x)}\right]\\
&= \frac{1}{dx'}\left[\delta(x'+dx'-x) - \delta(x'-x)\right]\\
&= \frac{1}{dx'}\left[\delta(x'-x+dx') - \delta(x'-x)\right]\\
&= \frac{\partial}{\partial x'}\delta(x'-x)
\end{aligned}}$$

$$\therefore \frac{\delta L}{\delta u(x)} = -\int_0^L g\,\frac{\partial u(x')}{\partial x'}\,\frac{\partial}{\partial x'}\delta(x'-x)\,dx'$$

$$= \int_0^L g\,\frac{\partial^2 u(x')}{\partial x'^2}\,\delta(x'-x)\,dx' \qquad \text{(by parts, surface term vanishes)}$$

$$= g\,\frac{\partial^2 u(x)}{\partial x^2}$$

Thus $\dfrac{d}{dt}\dfrac{\delta L}{\delta \dot{u}(x)} - \dfrac{\delta L}{\delta u(x)} = 0$

gives $\rho\ddot{u}(x) = g\dfrac{\partial^2 u(x)}{\partial x^2}$ as we wanted it to be!

Thus, the Lagrangian Equation is:

$$\boxed{\frac{d}{dt}\frac{\delta L}{\delta \dot{u}(x)} - \frac{\delta L}{\delta u(x)} = 0}^{+}$$

From this, we can define the momentum $\pi(x)$ conjugate to $u(x)$ by

$$\boxed{\pi(x) = \frac{\delta L}{\delta \dot{u}(x)}}$$

For the string,

$$\pi(x) = \rho \dot{u}(x)$$

Then one can construct the Hamiltonian via

$$\boxed{H = \int \dot{u}(x)\, \pi(x)\, dx - L} \quad \left(\text{c.f. } H = \sum_n \dot{u}_n p_n - L\right)$$

$$= \int \frac{\pi(x)^2}{\rho}\, dx - L$$

$$= \int_0^L \frac{\pi(x)^2}{2\rho}\, dx + \int_0^L \frac{g}{2}\left(\frac{\partial u(x)}{\partial x}\right)^2 dx$$

$$= \int_0^L \mathcal{H}(x)\, dx \qquad \mathcal{H}(x) = \text{Hamiltonian density}$$

+ There is an alternative (more popular) form that involves the Lagrangian density $\mathcal{L}$.

The Hamilton equations in continuum are

$$\dot{u}(x) = \frac{\delta H}{\delta \pi(x)} \quad ; \quad \dot{\pi}(x) = -\frac{\delta H}{\delta u(x)}$$

For the string,

$$\dot{u}(x) = \frac{1}{\rho}\pi(x) \quad \text{or} \quad \pi(x) = \rho\, \dot{u}(x)$$

and

$$\dot{\pi}(x) = g \frac{\partial^2 u(x)}{\partial x^2}$$

and hence the eq. of motion.

$\therefore$ It is possible to use Lagrangian and Hamiltonian formalism in a continuum, with the rules of differentiation modified.

Further Remark:

Recall:

$$L = \int_0^L \left[\frac{1}{2}\rho \dot{u}(x)^2 - \frac{1}{2} g \left(\frac{\partial u(x)}{\partial x}\right)^2\right] dx = \int_0^L \mathcal{L} \, dx$$

Lagrangian density

In general,

$$\mathcal{L}\left(u(\vec{x},t),\ \vec{\nabla} u(\vec{x},t),\ \frac{\partial}{\partial t} u(\vec{x},t)\right)$$

could also depend on higher derivatives, but usually first derivatives suffice.

useful in local field theories.

The Lagrange Equation in terms of $\mathcal{L}$ is:

$$\boxed{\frac{\partial \mathcal{L}}{\partial u(\vec{x},t)} - \vec{\nabla} \frac{\partial \mathcal{L}}{\partial(\vec{\nabla} u(\vec{x},t))} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial(\dot{u}(\vec{x},t))} = 0}$$

Example: For the string, $\frac{\partial \mathcal{L}}{\partial u(x)} = 0$, $\frac{\partial \mathcal{L}}{\partial \dot{u}} = \rho \dot{u} \Rightarrow \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{u}} = \rho \ddot{u}$

$$\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x}\right)} = -g\frac{\partial u}{\partial x} \Rightarrow \frac{\partial}{\partial x}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u}{\partial x}\right)}\right) = -g\frac{\partial^2 u}{\partial x^2}$$

$$\therefore \quad g\frac{\partial^2 u}{\partial x^2} - \rho \ddot{u} = 0$$

which is the eq. of motion.

This ends the introduction to classical field theory.

Continuum: Quantization of classical field

Promote $u(x) \rightarrow$ operator $u(x)$

$\pi(x) \rightarrow$ operator $\pi(x) = \frac{\hbar}{i}\frac{\delta}{\delta u(x)}$

$[\pi(x), u(x')] = ?$

$$\pi(x)\,u(x') - u(x')\,\pi(x)$$

$$= \frac{\hbar}{i}\left(\frac{\delta}{\delta u(x)}\,u(x') - u(x')\frac{\delta}{\delta u(x)}\right)$$

operating on an arbitrary function

$$= \frac{\hbar}{i}\left(u(x')\frac{\delta}{\delta u(x)} + \delta(x-x') - u(x')\frac{\delta}{\delta u(x)}\right)$$

$$= \frac{\hbar}{i}\,\delta(x-x')$$

$$\therefore\ [\pi(x), u(x')] = \frac{\hbar}{i}\,\delta(x-x')$$ +

Similarly, $[u(x), u(x')] = 0\ ;\ [\pi(x), \pi(x')] = 0$

We have H in terms of π and u. Thus, H also becomes an operator.

+ One can simply impose these commutation relations as the standard procedure in quantizing a classical field.

Recall:

$$u(x,t) = \sum_q \left(\frac{1}{\sqrt{L}} e^{iqx} B_q(t) + c.c. \right)$$

When $u(x,t)$ becomes an operator, so ~~are~~ $B_q(t)$ and $B_q^*(t)$.

$$\Pi(x,t) = \rho \dot{u}(x,t) = \sum_q \left(\frac{1}{\sqrt{L}} \rho(-i\omega(q)) e^{iqx} B_q(t) + c.c. \right)$$

We can look for $[B_q, B_{q'}^\dagger] = ?$

It is more convenient to define:

$$B_q = \sqrt{\frac{\hbar}{2\rho\omega(q)}}\, b_q \;;\quad B_q^\dagger = \sqrt{\frac{\hbar}{2\rho\omega(q)}}\, b_q^\dagger$$

Then,

$$u(x) = \sum_q \frac{1}{\sqrt{L}} \sqrt{\frac{\hbar}{2\rho\omega(q)}} \left(e^{iqx} b_q + e^{-iqx} b_q^\dagger \right)$$

$$\Pi(x) = \sum_q \frac{i}{\sqrt{L}} \sqrt{\frac{\hbar\omega(q)\rho}{2}} \left(-e^{iqx} b_q + e^{-iqx} b_q^\dagger \right)$$

In terms of $b_q, b_q^\dagger$, the Hamiltonian becomes

$$H = \sum_q \hbar\omega(q) \left(b_q^\dagger b_q + \frac{1}{2} \right)$$

The commutators of $b_q, b_{q'}^\dagger$ are

$$[b_q, b_{q'}^\dagger] = \delta_{qq'},\quad [b_q, b_{q'}] = 0,\quad [b_q^\dagger, b_{q'}^\dagger] = 0$$