# Connecting Particle and Field Mechanics

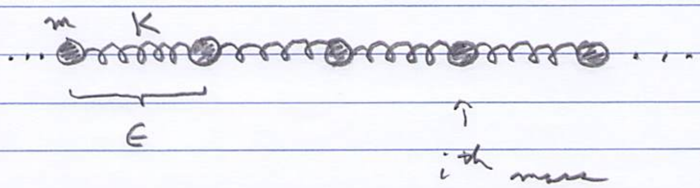
Consider the classical linear chain.

We have a linear chain of equal masses connected by springs of equal spring constant. The springs can oscillate about their equilibrium position in one dimension. In equilibrium, all masses are separated by an equal length.

$K \equiv$ value of the spring constant

$\epsilon \equiv$ length between the masses in equilibrium

$m \equiv$ mass of each of the coupled masses




(N masses in total)

Define

$\xi_n(t) =$ displacement of each oscillator from its equilibrium position $\bar{\xi}_n \equiv n\epsilon$ – i.e., $x_n(t) = n\epsilon + \xi_n(t)$

For simplicity, we will assume periodicity – i.e.,

$$\xi_1(t) = \xi_{N+1}(t)$$

In the limit $N \to \infty$, this will not matter.

The Lagrangian of this system is

$$\dot{x}_n(t) = \dot{q}_{\xi_n}(t) \qquad x_{n+1}(t) - x_n(t) - \epsilon$$

$$= (n+1)\epsilon + \xi_{n+1}(t) - n\epsilon - \xi_n(t) - \epsilon = \xi_{n+1}(t) - \xi_n(t)$$

$$L = T - V$$

$$= \frac{1}{2} m \sum_{n=1}^{N} \dot{q}_{\xi_n}^2 - \frac{1}{2} K \sum_{n=1}^{N} \underbrace{\left(q_{\xi_{n+1}} - \xi_n\right)}_{}^2$$

it's only the difference in the displacements of the masses from their equilibrium position that contributes to the potential energy

The Euler-Lagrange EOM for each mass are

$$\frac{\partial L}{\partial q_{\xi_n}} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_{\xi_n}}\right) = 0$$

$$\frac{\partial L}{\partial q_{\xi_n}} :$$

$$- \frac{1}{2} K \sum_{n=1}^{N} \left(q_{\xi_{n+1}} - \xi_n\right)^2$$

$$= - \frac{1}{2} K \Big[ (q_{\xi_2} - \xi_1)^2 + (q_{\xi_3} - q_{\xi_2})^2 + (q_{\xi_4} - \xi_3)^2 + \dots$$

$$\dots + (q_{\xi_n} - \xi_{n-1})^2 + (q_{\xi_{n+1}} - q_{\xi_n})^2 + \dots \Big]$$

Then

$$\frac{\partial L}{\partial q_{\xi_n}} = - \frac{1}{2} K \left[ 2(\xi_n - \xi_{n-1}) + 2(\xi_{n+1} - \xi_n)(-1) \right]$$

$$= - K \left( 2\xi_n - \xi_{n-1} - \xi_{n+1} \right)$$

$$= K\left(q_{n+1} - 2q_n + q_{n-1}\right)$$

$$\frac{\partial L}{\partial \dot{q}_n} = m\dot{q}_n$$

Then the EL EOM read

$$K\left(q_{n+1} - 2q_n + q_{n-1}\right) - m\ddot{q}_n = 0$$

We can compute the canonically conjugate momentum, $p_n$,

$$p_n = \frac{\partial L}{\partial \dot{q}_n} = m\dot{q}_n \quad \text{(as above)}$$

The Hamiltonian now follows

$$H = \sum_{n=1}^{N} p_n \dot{q}_n - L$$

$$= \sum_{n=1}^{N} p_n\left(\frac{p_n}{m}\right) - \left[\frac{1}{2}m\sum_{n=1}^{N}\left(\frac{p_n}{m}\right)^2 - \frac{1}{2}K\sum_{n=1}^{N}\left(q_{n+1} - q_n\right)^2\right]$$

$$= \sum_{n=1}^{N}\left[\frac{p_n^2}{m} - \frac{p_n^2}{2m} + \frac{1}{2}K\left(q_{n+1} - q_n\right)^2\right]$$

$$= \sum_{n=1}^{N}\frac{p_n^2}{2m} + \frac{1}{2}K\sum_{n=1}^{N}\left(q_{n+1} - q_n\right)^2$$

Finally, the Poisson Bracket is

$$\{q_n, p_{n'}\} = \sum_{n=1}^{N} \left( \frac{\partial q_n}{\partial q_k} \frac{\partial p_{n'}}{\partial p_k} - \frac{\partial q_n}{\partial p_k} \frac{\partial p_{n'}}{\partial q_k} \right)$$

$$= \sum_{n=1}^{N} \left( \delta_{nk} \delta_{n'k} \right)$$

$$= \delta_{nn} \delta_{n'n}$$

$$= \delta_{nn'}$$

Now we need to solve the EOM for $q_n(t)$.

Let

$$q_n(t) = q_n e^{i\omega t}$$

Then

$$-m q_n (i^2 \omega^2 e^{i\omega t}) + K(q_{n+1} - 2q_n + q_{n-1}) e^{i\omega t} = 0$$

or

$$(m\omega^2 - 2K) q_n + K(q_{n+1} + q_{n-1}) = 0$$

This has the solution

$$\xi_n = \frac{a_k}{\sqrt{N}} e^{ikna}$$

Inserting

$$(m\omega^2 - 2K)\frac{1}{\sqrt{N}} e^{ikna} + K\frac{1}{\sqrt{N}} e^{ikna}\left(e^{ika} + e^{-ika}\right) = 0$$

Then

$$(m\omega^2 - 2K) + 2K\cos ka = 0$$

This is the dispersion relation relating $\omega$ and $k$:

$$\omega^2 = \frac{1}{m} 2K(1-\cos ka) \Rightarrow \frac{4K}{m}\sin\left(\frac{ka}{2}\right) \Rightarrow \omega \pm$$

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or

$$\omega_k = \pm\left[\frac{2K}{m}(1-\cos ka)\right]^{1/2}$$

$$= \pm 2\sqrt{\frac{K}{m}}\sin\left(\frac{ka}{2}\right) \Rightarrow \omega_{-k} = -\omega_k \quad \text{where } \omega_k \equiv 2\sqrt{\frac{K}{m}}\sin\left(\frac{ka}{2}\right)$$

$k > 0$

Now let

$$\xi_n(t) = \xi_n^{\circ} e^{-i\omega t}$$

Then

$$-m q_n^* \left(i^2 \omega^2 e^{-i\omega t}\right) + K \left(q_{n+1}^* - 2 q_n^* + q_{n-1}^*\right) e^{-i\omega t} = 0$$

or

$$\left(m\omega^2 - 2K\right) q_n^* + K\left(q_{n+1}^* + q_{n-1}^*\right) = 0$$

which has the solution

$$q_n^* = \frac{a_k^*}{\sqrt{N}} e^{-ikna}$$

Inserting

$$\left(m\omega^2 - 2K\right) e^{-ikna} + K e^{-ikna}\left(e^{-ika} + e^{ika}\right) = 0$$

or

$$\left(m\omega^2 - 2K\right) + 2K \cos ka = 0$$

as before.

The general solution for $q_n(t)$ is then

$$q_n(t) = \frac{1}{\sqrt{N}} \sum_k \left(a_k e^{ikna} e^{i\omega_k t} + a_k^* e^{-ikna} e^{-i\omega_k t}\right)$$

To determine the values over which we sum $k$, recall that

$$q_1(0) = q_{N+1}(0)$$

which means that

$$\sum_k \left(e^{ika} + e^{-ika}\right) = \sum_k \left(e^{ik(N+1)a} + e^{-ik(N+1)a}\right)$$

Then

$$\sum_k \cos(ka) = \sum_k \cos[\overbrace{k(N+1)a}^{kNa+ka}]$$

$$= \sum_k \left(\cos kNa \cos ka - \sin kNa \sin ka\right)$$

which gives

$$\cos kNa = 1 \quad \Rightarrow kNa = 2\pi l \qquad l = \pm 1, \pm 2, \ldots$$

$$\sin kNa = 0$$

($l=0$ corresponds to a trivial solution)

$\lambda = \frac{2\pi}{k} = \frac{2\pi}{\frac{2\pi l}{Na}} = \frac{Na}{l}$

Then

$$q_n(t) = \frac{1}{\sqrt{N}} \sum_l \left(a_l e^{i2\pi l n/N} e^{i\omega_l t} + a_l^* e^{-i2\pi l n/N} e^{-i\omega_l t}\right)$$

$l \le \frac{N}{2}$

$\Rightarrow \lambda \ge 2a$

$$\equiv \sum_l \left[u_{n,l}\, a_l(t) + u_{n,l}^*\, a_l^*(t)\right]$$

where $u_{n,l} = \frac{1}{\sqrt{N}} e^{i2\pi l n/N}$

$a_l(t) = a_l e^{i\omega_l t}$

To determine the limits of $l$ note that the smallest wave-length that can fit on our chain is

$$\lambda_{minimum} = 2a$$

since

$$\lambda = \frac{2\pi}{k}$$

$$= \frac{2\pi}{\frac{2\pi l}{Na}}$$

$$= \frac{Na}{l}$$

we have

$$\lambda_{min} = \frac{Na}{l_{max}}$$

$$= 2a$$

Then

$$l_{max} = \frac{N}{2}$$

and our sum over $l$ becomes

$$q_n(t) = \sum_{l=-\frac{N}{2}}^{+\frac{N}{2}} \left[ a_l(t) u_{n,l} + a_l^*(t) u_{n,l}^* \right]$$

Now compute $q_n(t)$:

$$p_n(t) = m\dot{q}_n(t)$$

$$= m \sum_{l=-\frac{N}{2}}^{+\frac{N}{2}} i\omega_l \left[ a_l(t)\, u_{n,l} - a_l^*(t)\, u^*_{n,l} \right]$$

Let's now compute the Hamiltonian:

$$H = \frac{1}{2m}\sum_{n=1}^{N} p_n^2 + \frac{1}{2}K\sum_{n=1}^{N}(q_{n+1}-q_n)^2$$

$$T = \sum_{n=1}^{N} \frac{p_n^2}{2m}$$

$$= -\frac{m}{2}\sum_n \left\{ \left[ \sum_l \omega_l (a_l u_{n,l} - a_l^* u^*_{n,l}) \right] \left[ \sum_{l'} \omega_{l'} (a_{l'} u_{n,l'} - a^*_{l'} u^*_{n,l'}) \right] \right\}$$

$$= -\frac{m}{2}\sum_n \left\{ \sum_{ll'} \omega_l \omega_{l'} \left( a_l a_{l'} u_{n,l} u_{n,l'} - a_l a^*_{l'} u_{n,l} u^*_{n,l'} \right.\right.$$

$$\left.\left. - a^*_l a_{l'} u^*_{n,l} u_{n,l'} + a^*_l a^*_{l'} u^*_{n,l} u^*_{n,l'} \right) \right\}$$

The orthonormality of the basis functions $u_{n,l}$ tells us that

$$\sum_{n=1}^{N} u^*_{n,l'} u_{n,l} = \delta_{ll'}$$

$$\sum_{n=1}^{N} u_{n,l'} u_{n,l} = \delta_{l,-l'}$$

$$\sum_{n=1}^{N} u^*_{n,l'} u^*_{n,l} = \delta_{l,-l'}$$

Then

$$T = -\frac{m}{2}\sum_{\ell\ell'}\omega_\ell\omega_{\ell'}\left(a_\ell a_{\ell'}\delta_{\ell,-\ell'} - a_\ell a^*_{\ell'}\delta_{\ell\ell'}\right.$$
$$\left. - a^*_\ell a_{\ell'}\delta_{\ell\ell'} + a^*_\ell a^*_{\ell'}\delta_{\ell,-\ell'}\right)$$

$$= -\frac{m}{2}\sum_\ell\left(\omega_\ell\underbrace{\omega_{-\ell}}_{=\omega_\ell} a_\ell a_{-\ell} - \omega_\ell^2 a_\ell a^*_\ell - \omega_\ell^2 a^*_\ell a_\ell + \omega_\ell\omega_{-\ell} a^*_\ell a^*_{-\ell}\right)$$

$$= -\frac{m}{2}\sum_\ell\omega_\ell^2\left(a_\ell a_{-\ell} - a_\ell a^*_\ell - a^*_\ell a_\ell + a^*_\ell a^*_{-\ell}\right)$$

$$= -\frac{m}{2}\sum_\ell\omega_\ell^2\left(a_\ell e^{i\omega_\ell t} a_{-\ell} e^{i\omega_{-\ell} t} - a_\ell e^{i\omega_\ell t} a^*_\ell e^{-i\omega_\ell t}\right.$$
$$\left. - a^*_\ell e^{-i\omega_\ell t} a_\ell e^{i\omega_\ell t} + a^*_\ell e^{-i\omega_\ell t} a^*_{-\ell} e^{-i\omega_{-\ell} t}\right)$$

$$= -\frac{m}{2}\sum_\ell\omega_\ell^2\left(a_\ell a_{-\ell} e^{2i\omega_\ell t} - a_\ell a^*_\ell - a^*_\ell a_\ell + a^*_\ell a^*_{-\ell} e^{-2i\omega_\ell t}\right)$$

Now let's compute

$$V = \frac{1}{2}K\sum_{n=1}^{N}\left(q_{n+1} - q_n\right)^2$$

$$= \frac{1}{2}K\sum_n\left\{\sum_\ell\left[\left(a_\ell u_{n+1,\ell} + a^*_\ell u^*_{n+1,\ell}\right) - \left(a_\ell u_{n,\ell} + a^*_\ell u^*_{n,\ell}\right)\right]\right\}^2$$

$$= \frac{1}{2}K\sum_n\sum_\ell\sum_{\ell'}\left\{\left(a_\ell u_{n+1,\ell} + a^*_\ell u^*_{n+1,\ell}\right)\left(a_{\ell'} u_{n+1,\ell'} + a^*_{\ell'} u^*_{n+1,\ell'}\right)\right.$$

$$+\left(a_{l}u_{n,l}+a^{*}_{l}u^{*}_{n,l}\right)\left(a_{l'}u_{n,l'}+a^{*}_{l'}u^{*}_{n,l'}\right)$$

$$-\left(a_{l}u_{n+1,l}+a^{*}_{l}u^{*}_{n+1,l}\right)\left(a_{l'}u_{n,l'}+a^{*}_{l'}u^{*}_{n,l'}\right)$$

$$-\left(a_{l}u_{n,l}+a^{*}_{l}u^{*}_{n,l}\right)\left(a_{l'}u_{n+1,l'}+a^{*}_{l'}u^{*}_{n+1,l'}\right)\Big\}$$

$$=\frac{1}{2}K\sum_{n}\sum_{l}\sum_{l'}\Big\{\left(a_{l}e^{i2\pi l/N}u_{n,l}+a^{*}_{l}e^{-i2\pi l/N}u^{*}_{n,l}\right)\left(a_{l'}e^{i2\pi l'/N}u_{n,l'}+a^{*}_{l'}e^{-i2\pi l'/N}u^{*}_{n,l'}\right)$$

$$+\left(a_{l}u_{n,l}+a^{*}_{l}u^{*}_{n,l}\right)\left(a_{l'}u_{n,l'}+a^{*}_{l'}u^{*}_{n,l'}\right)$$

$$-\left(a_{l}e^{i2\pi l/N}u_{n,l}+a^{*}_{l}e^{-i2\pi l/N}u^{*}_{n,l}\right)\left(a_{l'}u_{n,l'}+a^{*}_{l'}u^{*}_{n,l'}\right)$$

$$-\left(a_{l}u_{n,l}+a^{*}_{l}u^{*}_{n,l}\right)\left(a_{l'}e^{i2\pi l'/N}u_{n,l'}+a^{*}_{l'}e^{-i2\pi l'/N}u^{*}_{n,l'}\right)\Big\}$$

$$=\frac{1}{2}K\sum_{l}\sum_{l'}\Big\{a_{l}a_{l'}e^{i2\pi l/N}e^{i2\pi l'/N}\delta_{l,-l'}+a_{l}a^{*}_{l'}e^{i2\pi l/N}e^{-i2\pi l'/N}\delta_{l,l'}$$

$$+a^{*}_{l}a_{l'}e^{-i2\pi l/N}e^{i2\pi l'/N}\delta_{l,l'}+a^{*}_{l}a^{*}_{l'}e^{-i2\pi l/N}e^{-i2\pi l'/N}\delta_{l,-l'}$$

$$+a_{l}a_{l'}\delta_{l,-l'}+a_{l}a^{*}_{l'}\delta_{l,l'}+a^{*}_{l}a_{l'}\delta_{l,l'}+a^{*}_{l}a^{*}_{l'}\delta_{l,-l'}$$

$$-a_{l}a_{l'}e^{i2\pi l/N}\delta_{l,-l'}-a_{l}a^{*}_{l'}e^{i2\pi l/N}\delta_{l,l'}$$

$$-a^{*}_{l}a_{l'}e^{-i2\pi l/N}\delta_{l,l'}-a^{*}_{l}a^{*}_{l'}e^{-i2\pi l/N}\delta_{l,-l'}$$

$$-a_{l}a_{l'}e^{i2\pi l'/N}\delta_{l,-l'}-a_{l}a^{*}_{l'}e^{-i2\pi l'/N}\delta_{l,l'}$$

$$- a^*_{l} a_{l'} e^{i 2\pi l'/N} \delta_{l,l'} - a^*_{l} a^*_{l'} e^{-i 2\pi l'/N} \delta_{l,-l'} \Big\}$$

$$= \tfrac{1}{2} K \sum_{l} \Big\{ a_{l} a_{-l} + a_{l} a^*_{l} + a^*_{l} a_{l} + a^*_{l} a^*_{-l}$$

$$+ a_{l} a_{-l} + a_{l} a^*_{l} + a^*_{l} a_{l} + a^*_{l} a^*_{-l}$$

$$- a_{l} a_{-l} e^{i 2\pi l/N} - a_{l} a^*_{l} e^{i 2\pi l/N}$$

$$- a^*_{l} a_{l} e^{-i 2\pi l/N} - a^*_{l} a^*_{-l} e^{-i 2\pi l/N}$$

$$- a_{l} a_{-l} e^{-i 2\pi l/N} - a_{l} a^*_{l} e^{-i 2\pi l/N}$$

$$- a^*_{l} a_{l} e^{i 2\pi l/N} - a^*_{l} a^*_{-l} e^{i 2\pi l/N} \Big\}$$

$$= \tfrac{1}{2} K \sum_{l} \Big\{ a_{l} a_{-l} \left[ 2 - \left( e^{i 2\pi l/N} + e^{-i 2\pi l/N} \right) \right]$$

$$+ a_{l} a^*_{l} \left[ 2 - \left( e^{i 2\pi l/N} + e^{-i 2\pi l/N} \right) \right]$$

$$+ a^*_{l} a_{l} \left[ 2 - \left( e^{i 2\pi l/N} + e^{-i 2\pi l/N} \right) \right]$$

$$+ a^*_{l} a^*_{-l} \left[ 2 - \left( e^{i 2\pi l/N} + e^{-i 2\pi l/N} \right) \right] \Big\}$$

$$= K \sum_{l} \left( a_{l} a_{-l} + a_{l} a^*_{l} + a^*_{l} a_{l} + a^*_{l} a^*_{-l} \right) \underbrace{\left( 1 - \cos \frac{2\pi l}{N} \right)}_{1 - \cos(ka)}$$

But

$$\frac{m\omega^2}{2K} = 1 - \cos(ka)$$

Then

$$V = \frac{m}{2}\sum_l \omega_l^2 \left( a_l a_{-l} e^{2i\omega_l t} + a_l a_l^* + a_l^* a_l + a_l^* a_{-l}^* e^{-2i\omega_l t} \right)$$

Finally

$$H = T + V$$

$$= -\frac{m}{2}\sum_l \omega_l^2 \left( a_l a_{-l} e^{2i\omega_l t} - a_l a_l^* - a_l^* a_l + a_l^* a_{-l}^* e^{-2i\omega_l t} \right)$$

$$+ \frac{m}{2}\sum_l \omega_l^2 \left( a_l a_{-l} e^{2i\omega_l t} + a_l a_l^* + a_l^* a_l + a_l^* a_{-l}^* e^{-2i\omega_l t} \right)$$

$$= \sum_l m\omega_l^2 \left( a_l^* a_l + a_l a_l^* \right)$$

But this is the Hamiltonian for a collection of uncoupled oscillators, each one corresponding to a different normal mode of the system.

When we quantize this system, the quanta of the modes will correspond to the quasi-particles known as phonons.