Connecting Particle and Field Mechanics

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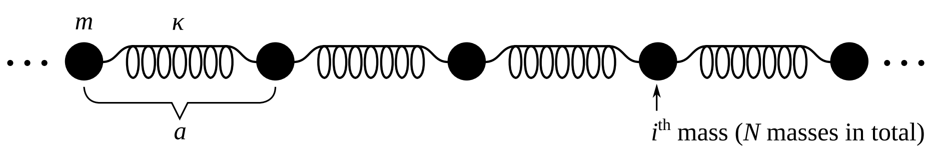
Consider we have a classical linear chain of equal masses connected by spring of equal spring constant. The springs can oscillate about there equilibrium position in one dimension. In equilibrium all masses are separated by an equal length.

$\kappa =$ value of the spring constant

$a =$ length between the masses in equilibrium

$m =$ mass of each of the sampled masses



Define

$q_n(t) =$ displacement of each oscillator from its equilibrium position $\bar{q}_n \equiv na$ – i.e., $x_n(t) = na + q_n(t)$

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

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

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

The Lagrangian of this system is

$$\begin{aligned} L &= T - V \\ &= \frac{1}{2} m \sum_{n=1}^{N} \dot{q}_n^2 - \frac{1}{2}\kappa \sum_{n=1}^{N} \underbrace{\left(q_{n+1} - q_n\right)^2} \end{aligned}$$

$\boxed{\dot{x}_n(t) = \dot{q}_n(t)}$

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

$$\begin{aligned} \big(x_{n+1}(t) - x_n(t)\big) - a &= (n+1)a + q_{n+1}(t) \\ &\quad - na - q_n(t) - a \\ &= q_{n+1}(t) - q_n(t) \end{aligned}$$

The Euler-Lagrangian EOM for each mass are

$$\frac{\partial L}{\partial q_n} - \frac{d}{\mathrm{d}t}\left[\frac{\partial L}{\partial \dot{q}_n}\right] = 0 \tag{1}$$

$\dfrac{\partial L}{\partial q_n}$:

$$\begin{aligned}
&-\tfrac{1}{2}\kappa\sum_{n=1}^{N}(q_{n+1}-q_n)^2\\
&= -\tfrac{1}{2}\kappa\left[(q_2-q_1)^2) + (q_3-q_2)^2 + (q_4-q_3)^2 + \dots\right.\\
&\qquad\left. +(q_n-q_{n-1})^2 + (q_{n+1}-q_n)^2 + \dots\right]
\end{aligned}$$

Then

$$\begin{aligned}
\frac{\partial L}{\partial q_n} &= -\tfrac{1}{2}\kappa\left[2(q_n-q_{n-1}) + 2(q_{n+1}-q_n)(-1)\right]\\
&= -\kappa\left[2q_n - q_{n-1} - q_{n+1}\right]
\end{aligned}$$

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

Then the Euler-Lagrange EOM read

$$\kappa\left[q_{n+1} - 2q_n + q_{n-1}\right] - m\ddot{q}_n = 0$$

We can compute the canonically conjugate momentum, p_n,

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

The Hamiltonian now follows

$$\begin{aligned}
H &= \sum_{n=1}^{N} p_n\dot{q}_n - L\\
&= \sum_{n=1}^{N} p_n\frac{p_n}{m} - \left[\frac{1}{2}m\sum_{n=1}^{N}\left(\frac{p_n}{m}\right)^2 - \tfrac{1}{2}\kappa\sum_{n=1}^{N}(q_{n+1}-q_n)^2\right]\\
&= \sum_{n=1}^{N}\left[\frac{p_n^2}{m} - \frac{p_n^2}{2m} + \tfrac{1}{2}\kappa(q_{n+1}-q_n)^2\right]\\
&= \sum_{n=1}^{N}\frac{p_n^2}{2m} + \tfrac{1}{2}\kappa\sum_{n=1}^{N}(q_{n+1}-q_n)^2
\end{aligned}$$

Finally, the Poisson Bracket is

$$
\begin{aligned}
\{q_n, p_{n'}\} &= \sum_{n=1}^{N} \left(\frac{\partial q_n}{\partial q_k} \frac{\partial p_{n'}}{\partial p_k} - \frac{\partial q_n}{\partial p_k} \frac{\partial p_{n'}}{\partial q_k} \right) \\
&= \sum_{n=1}^{N} \left(\delta_{nk} \delta_{n'k} \right) \\
&= \delta_{nn} \delta_{n'n} \\
&= \delta_{nn'}
\end{aligned}
$$

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

Let

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

Then

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

or

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

This has the solution

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

Inserting

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

Then

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

This is the dispersion relation relating ω and k:

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

or

$$
\begin{aligned}
\omega_k &= \pm \left[\frac{2\kappa}{m} \left(1 - \cos(ka) \right) \right]^{\frac{1}{2}} \\
&= \pm 2 \sqrt{\frac{\kappa}{m}} \sin \left(\frac{ka}{2} \right) \qquad \Longrightarrow \qquad \omega_{-k} = \omega_k \text{ where } \omega_k \equiv 2 \sqrt{\frac{\kappa}{m}} \sin \left(\frac{ka}{2} \right), k > 0
\end{aligned}
$$

Now let

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

Then

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

or

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

which has the solution

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

Inserting

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

or

$$\left(m\omega^2 - 2\kappa\right) + 2\kappa \cos(ka)$$

as before.

The general relation 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

$$\begin{aligned}
\sum_k \cos(ka) &= \sum_k \cos[\underbrace{k(N+1)a}_{kNa+ka}] \\
&= \sum_k \left(\cos(kNa)\cos(ka) - \sin(kNa)\sin(ka)\right)
\end{aligned}$$

which gives

$$\begin{array}{lcll}
\cos(kNa) = 1 & \Longrightarrow & kNa = 2\pi l & l = \pm 1, \pm 2, \ldots \\
\sin(kNa) = 0 & & \multicolumn{2}{l}{(l = 0 \text{ corresponds to a trivial solution})}
\end{array}$$

Then

$$\begin{aligned} q_n(t) &= \frac{1}{\sqrt{N}} \sum_l \left(a_l e^{i\frac{2\pi l n}{N}} e^{i\omega_l t} + a_l^* e^{-i\frac{2\pi l n}{N}} e^{-i\omega_l t} \right) \\ &= \sum_l \left[u_{n,l} a_l(t) + u_{n,l}^* a_l^*(t) \right] \end{aligned}$$

where

$$\begin{aligned} u_{n,l} &= \frac{1}{\sqrt{N}} e^{i\frac{2\pi l n}{N}} \\ a_l(t) &= a_l e^{i\omega_l t} \end{aligned}$$

To determine the limits of l, note that the smallest wavelength that can fit on our chain is

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

Since

$$\begin{aligned} \lambda &= \frac{2\pi}{k} \\ &= \frac{2\pi}{\frac{2\pi l}{Na}} \\ &= \frac{Na}{l} \end{aligned}$$

we have

$$\begin{aligned} \lambda_{\text{min}} &= \frac{Na}{l_{\text{max}}} \\ &= 2a \end{aligned}$$

Then

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

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 $p_n(t)$:

$$\begin{aligned} p_n(t) &= m\dot{q}_n(t) \\ &= m \sum_{l=-\frac{N}{2}}^{+\frac{N}{2}} i\omega_l \left[a_l(t) u_{n,l} - a_l^*(t) u_{n,l}^* \right] \end{aligned}$$

Let's now compute the Hamiltonian:

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

$$\begin{aligned}
T &= \sum_{n=1}^{N} \frac{p_n^2}{2m} \\
&= -\frac{m}{2}\sum_n \left\{ \left[\omega_l \left(a_l(t)u_{n,l} - a_l^*(t)u_{n,l}^*\right)\right]\left[\omega_{l'}\left(a_{l'}(t)u_{n,l'} - a_{l'}^*(t)u_{n,l'}^*\right)\right]\right\} \\
&= -\frac{m}{2}\sum_n \Bigg\{ \sum_{ll'} \omega_l\omega_{l'} \Big(a_l(t)a_{l'}(t)u_{n,l}u_{n,l'} - a_l(t)a_{l'}^*(t)u_{n,l}u_{n,l'}^* \\
&\qquad\qquad - a_l^*(t)a_{l'}(t)u_{n,l}^*u_{n,l'} + a_l(t)^* a_{l'}^*(t)u_{n,l}^*u_{n,l'}^* \Big)\Bigg\}
\end{aligned}$$

The orthogonality 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

$$\begin{aligned}
T &= -\frac{m}{2}\sum_{ll'} \omega_l\omega_{l'} \Big(a_l(t)a_{l'}(t)\delta_{l,-l'} - a_l(t)a_{l'}^*(t)\delta_{ll'} \\
&\qquad - a_l^*(t)a_{l'}(t)\delta_{ll'} + a_l(t)^* a_{l'}^*(t)\delta_{l,-l'}\Big) \\
&= -\frac{m}{2}\sum_l \Big(\omega_l \underbrace{\omega_{-l}}_{=\omega_l} a_l(t)a_{-l}(t) - \omega_l^2 a_l(t)a_l^*(t) - \omega_l^2 a_l^*(t)a_l(t) + \omega_l \underbrace{\omega_{-l}}_{=\omega_l} a_l^*(t)a_{-l}^*(t)\Big) \\
&= -\frac{m}{2}\sum_l \omega_l^2 \Big(a_l(t)a_{-l}(t) - a_l(t)a_l^*(t) - a_l^*(t)a_l(t) + a_l^*(t)a_{-l}^*(t)\Big) \\
&= -\frac{m}{2}\sum_l \omega_l^2 \Big(a_l e^{i\omega_l t} a_{-l}e^{i\omega_{-l}t} - a_l e^{i\omega_l t} a_l^* e^{-i\omega_l t} \\
&\qquad - a_l^* e^{-i\omega_l t} a_l e^{i\omega_l t} + a_l^* e^{-i\omega_l t} a_{-l}^* e^{-i\omega_{-l}t}\Big) \\
&= -\frac{m}{2}\sum_l \omega_l^2 \Big(a_l a_{-l} e^{2i\omega_l t} - a_l a_l^* - a_l^* a_l + a_l^* a_{-l}^* e^{-2i\omega_l t}\Big)
\end{aligned}$$

Now let's compute

$$
\begin{aligned}
V &= \frac{1}{2}\kappa \sum_{n=1}^{N} \left(q_{n+1} - q_n\right)^2 \\
&= \frac{1}{2}\kappa \sum_{n} \Big\{ \sum_{l} \big[\left(a_l(t) u_{n+1,l} + a_l^*(t) u_{n+1,l}^*\right) - \left(a_l(t) u_{n,l} + a_l^*(t) u_{n,l}^*\right) \big] \Big\}^2 \\
&= \frac{1}{2}\kappa \sum_{n}\sum_{l}\sum_{l'} \Big\{ \left(a_l(t) u_{n+1,l} + a_l^*(t) u_{n+1,l}^*\right) \left(a_{l'}(t) u_{n+1,l'} + a_{l'}^*(t) u_{n+1,l'}^*\right) \\
&\qquad + \left(a_l(t) u_{n,l} + a_l^*(t) u_{n,l}^*\right) \left(a_{l'}(t) u_{n,l'} + a_{l'}^*(t) u_{n,l'}^*\right) \\
&\qquad - \left(a_l(t) u_{n+1,l} + a_l^*(t) u_{n+1,l}^*\right) \left(a_{l'}(t) u_{n,l'} + a_{l'}^*(t) u_{n,l'}^*\right) \\
&\qquad - \left(a_l(t) u_{n,l} + a_l^*(t) u_{n,l}^*\right) \left(a_{l'}(t) u_{n+1,l'} + a_{l'}^*(t) u_{n+1,l'}^*\right) \Big\} \\
&= \frac{1}{2}\kappa \sum_{n}\sum_{l}\sum_{l'} \Big\{ \left(a_l(t) e^{i\frac{2\pi l}{N}} u_{n,l} + a_l^*(t) e^{-i\frac{2\pi l}{N}} u_{n,l}^*\right) \left(a_{l'}(t) e^{i\frac{2\pi l'}{N}} u_{n,l'} + a_{l'}^*(t) e^{-i\frac{2\pi l'}{N}} u_{n,l'}^*\right) \\
&\qquad + \left(a_l(t) u_{n,l} + a_l^*(t) u_{n,l}^*\right) \left(a_{l'}(t) u_{n,l'} + a_{l'}^*(t) u_{n,l'}^*\right) \\
&\qquad - \left(a_l(t) e^{i\frac{2\pi l}{N}} u_{n,l} + a_l^*(t) e^{-i\frac{2\pi l}{N}} u_{n,l}^*\right) \left(a_{l'}(t) u_{n,l'} + a_{l'}^*(t) u_{n,l'}^*\right) \\
&\qquad - \left(a_l(t) u_{n,l} + a_l^*(t) u_{n,l}^*\right) \left(a_{l'}(t) e^{i\frac{2\pi l'}{N}} u_{n,l'} + a_{l'}^*(t) e^{-i\frac{2\pi l'}{N}} u_{n,l'}^*\right) \Big\} \\
&= \frac{1}{2}\kappa \sum_{l}\sum_{l'} \Big\{ a_l(t) a_{l'}(t) e^{i\frac{2\pi l}{N}} e^{i\frac{2\pi l'}{N}} \delta_{l,-l'} + a_l(t) a_{l'}^*(t) e^{i\frac{2\pi l}{N}} e^{-i\frac{2\pi l'}{N}} \delta_{l,l'} \\
&\qquad + a_l^*(t) a_{l'}(t) e^{-i\frac{2\pi l}{N}} e^{i\frac{2\pi l'}{N}} \delta_{l,l'} + a_l^*(t) a_{l'}^* e^{-i\frac{2\pi l}{N}} e^{-i\frac{2\pi l'}{N}} \delta_{l,-l'} \\
&\qquad + a_l(t) a_{l'}(t) \delta_{l,-l'} + a_l(t) a_{l'}^*(t) \delta_{l,l'} + a_l^*(t) a_{l'}(t) \delta_{l,l'} + a_l^*(t) a_{l'}^*(t) \delta_{l,-l'} \\
&\qquad - a_l(t) a_{l'}(t) e^{i\frac{2\pi l}{N}} \delta_{l,-l'} - a_l(t) a_{l'}^*(t) e^{i\frac{2\pi l}{N}} \delta_{l,l'} \\
&\qquad - a_l^*(t) a_{l'}(t) e^{-i\frac{2\pi l}{N}} \delta_{l,l'} - a_l^*(t) a_{l'}^*(t) e^{-i\frac{2\pi l}{N}} \delta_{l,-l'} \\
&\qquad - a_l(t) a_{l'}(t) e^{i\frac{2\pi l'}{N}} \delta_{l,-l'} - a_l(t) a_{l'}^*(t) e^{-i\frac{2\pi l'}{N}} \delta_{l,l'} \\
&\qquad - a_l^*(t) a_{l'}(t) e^{i\frac{2\pi l'}{N}} \delta_{l,l'} - a_l^*(t) a_{l'}^*(t) e^{-i\frac{2\pi l'}{N}} \delta_{l,-l'} \Big\} \\
&= \frac{1}{2}\kappa \sum_{l} \Big\{ a_l(t) a_{-l}(t) + a_l(t) a_l^*(t) + a_l^*(t) a_l(t) + a_l^*(t) a_{-l}^*(t) \\
&\qquad + a_l(t) a_{-l}(t) + a_l(t) a_l^*(t) + a_l^*(t) a_l(t) + a_l^*(t) a_{-l}^*(t) \\
&\qquad - a_l(t) a_{-l}(t) e^{i\frac{2\pi l}{N}} - a_l(t) a_l^*(t) e^{i\frac{2\pi l}{N}} \\
&\qquad - a_l^*(t) a_l(t) e^{-i\frac{2\pi l}{N}} - a_l^*(t) a_{-l}^*(t) e^{-i\frac{2\pi l}{N}} \\
&\qquad - a_l(t) a_{-l}(t) e^{-i\frac{2\pi l}{N}} - a_l(t) a_l^*(t) e^{-i\frac{2\pi l}{N}} \\
&\qquad - a_l^*(t) a_l(t) e^{i\frac{2\pi l}{N}} - a_l^*(t) a_{-l}^*(t) e^{i\frac{2\pi l}{N}} \Big\}
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2}\kappa \sum_l \Big\{ a_l(t)a_{-l}(t)\left[2 - \left(e^{i\frac{2\pi l}{N}} + e^{-i\frac{2\pi l}{N}}\right)\right] \\
&\qquad\qquad + a_l(t)a_l^*(t)\left[2 - \left(e^{i\frac{2\pi l}{N}} + e^{-i\frac{2\pi l}{N}}\right)\right] \\
&\qquad\qquad + a_l^*(t)a_l(t)\left[2 - \left(e^{i\frac{2\pi l}{N}} + e^{-i\frac{2\pi l}{N}}\right)\right] \\
&\qquad\qquad + a_l^*(t)a_{-l}^*(t)\left[2 - \left(e^{i\frac{2\pi l}{N}} + e^{-i\frac{2\pi l}{N}}\right)\right] \Big\} \\
&= \kappa \sum_l \left(a_l(t)a_{-l}(t) + a_l(t)a_l^*(t) + a_l^*(t)a_l(t) + a_l^*(t)a_{-l}^*(t)\right)\left(\underbrace{1 - \cos\left(\tfrac{2\pi l}{N}\right)}_{1-\cos(ka)}\right)
\end{aligned}
$$

But

$$
\frac{m\omega_k^2}{2\kappa} = 1 - \cos(ka)
$$

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

$$
\begin{aligned}
H &= T + V \\
&= -\frac{m}{2}\sum_l \omega_l^2\left(a_l a_{-l}e^{2i\omega_l t} - a_l a_l^* - a_l^* a_l + a_l^* a_{-l}^* e^{-2i\omega_l t}\right) \\
&\quad + \frac{m}{2}\sum_l \omega_l^2\left(a_l a_{-l}e^{2i\omega_l t} + a_l a_l^* + a_l^* a_l + a_l^* a_{-l}^* e^{-2i\omega_l t}\right) \\
&= \sum_l m\omega_l^2\left(a_l^* a_l + a_l a_l^*\right)
\end{aligned}
$$

But this is the Hamiltonian for a collection of <u>uncoupled</u> 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 <u>quasi-particles</u> known as <u>phonons</u>.