LINEAR CHAIN OF OSCILLATORS - CLASSICAL TREATMENT, EQUATIONS OF MOTION

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Reference: W. Greiner & J. Reinhardt, *Field Quantization*, Springer-Verlag (1996), Section 1.4.

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Greiner studies a generalization of the system of two coupled masses on springs that we looked at in Shankar's book. Consider a chain of N masses m connected by springs, all of which have rest length a and spring constant κ. The displacement of mass n from its equilibrium position is $q_n(t)$. Thus the length of spring n is given by $q_{n+1}(t)-q_n(t)$, so the potential energy of spring n is $\frac{1}{2}\kappa\left(q_{n+1}(t)-q_n(t)\right)^2$, according to the standard recipe for a harmonic oscillator. The Lagrangian is therefore

$$L = T - V \tag{1}$$

$$= \frac{1}{2}m\sum_{n=1}^{N}\dot{q}_n^2 - \frac{\kappa}{2}\sum_{n=1}^{N}\left(q_{n+1}(t)-q_n(t)\right)^2 \tag{2}$$

The Hamiltonian is

$$H = T + V \tag{3}$$

$$= \frac{1}{2}m\sum_{n=1}^{N}\dot{q}_n^2 + \frac{\kappa}{2}\sum_{n=1}^{N}\left(q_{n+1}(t)-q_n(t)\right)^2 \tag{4}$$

Using the Euler-Lagrange equations leads to the equations of motion

$$m\ddot{q}_n = \kappa\left(q_{n+1}+q_{n-1}-2q_n\right) \tag{5}$$

This is a set of coupled second-order differential equations which, as it stands, would be difficult to solve by brute force. To solve any differential equation we need to specify boundary conditions; Greiner uses periodic boundary conditions, which means that we require

$$q_{N+1}(t) = q_1(t) \tag{6}$$

This is roughly equivalent to connecting the two ends of the chain together to form a loop, although doing this with a real system of masses on springs would introduce bends in the springs which we aren't considering.

To decouple the equations, we introduce normal coordinates, which is done by expanding each coordinate function in a series

$$q_n(t) = \sum_k a_k(t)\, u_n^k \tag{7}$$

Note that k in u_n^k is an index, not an exponent.

Choosing

$$u_n^k = \frac{1}{\sqrt{N}} e^{ikan} \tag{8}$$

and imposing the periodic boundary conditions leads to a discrete Fourier transform. The boundary condition requires $u_{N+n}^k = u_n^k$, which means that $e^{ikaN} = 1$.

Thus k is restricted to

$$k = \frac{2\pi}{Na} l \tag{9}$$

where l is an integer. In practice, l can take on any range that covers N consecutive integers; Greiner chooses

$$-\frac{N}{2} < l \le \frac{N}{2} \tag{10}$$

Using a value of l outside this range results in a linear combination of the functions within the range. For example, if we choose $l = \frac{N}{2} + 1$, then

$$e^{2\pi i(N/2+1)an/Na} = e^{i\pi n} e^{2\pi in/N} \tag{11}$$

$$= (-1)^n e^{2\pi in/N} \tag{12}$$

where $e^{2\pi in/N}$ is u_n^k with $l = 1$.

Greiner proves (eqns 1.64 - 1.66) a couple of useful identities:

$$\sum_{n=1}^{N} u_n^{k'*} u_n^k = \delta_{kk'} \tag{13}$$

$$\sum_{k=1}^{N} u_{n'}^{k*} u_n^k = \delta_{nn'} \tag{14}$$

From its definition 8, we see that

$$u_n^{k*} = u_n^{-k} \tag{15}$$

The coordinates q_n in 7 must be real, so we have

$$q_n^* = \sum_k a_k^*(t)\, u_n^{k*} \tag{16}$$
$$= \sum_k a_k^*(t)\, u_n^{-k} \tag{17}$$
$$= q_n \tag{18}$$

Since we're taking k to be over a range symmetric about $k=0$, we can replace the sum over k by a sum over $-k$, which means that

$$a_k^*(t) = a_{-k}(t) \tag{19}$$

The benefit of using the decomposition 7 is that we can decouple the differential equations. To see this, we plug 7 into 5:

$$m\sum_{k'} \ddot{a}_{k'}(t)\, u_n^{k'} = \kappa \sum_{k'} a_{k'}(t)\left(u_{n+1}^{k'} + u_{n-1}^{k'} - 2u_n^{k'}\right) \tag{20}$$

We can multiply by u_n^{k*} and sum over n:

$$m\sum_{k'} \ddot{a}_{k'}(t) \sum_n u_n^{k*} u_n^{k'} = \kappa \sum_{k'} a_{k'}(t) \sum_n u_n^{k*}\left(u_{n+1}^{k'} + u_{n-1}^{k'} - 2u_n^{k'}\right) \tag{21}$$

Using 13 on the LHS, we get

$$m\sum_{k'} \ddot{a}_{k'}(t)\, \delta_{kk'} = \kappa \sum_{k'} a_{k'}(t) \sum_n u_n^{k*}\left(u_{n+1}^{k'} + u_{n-1}^{k'} - 2u_n^{k'}\right) \tag{22}$$
$$m\ddot{a}_k(t) = \kappa \sum_{k'} a_{k'}(t) \sum_n u_n^{k*}\left(u_{n+1}^{k'} + u_{n-1}^{k'} - 2u_n^{k'}\right) \tag{23}$$

From the definition 8

$$u_{n\pm 1}^k = e^{\pm ika} u_n^k \tag{24}$$

Inserting this into 23 and using 13 again:

$$m\ddot{a}_k(t) = \kappa \sum_{k'} a_{k'}(t) \sum_n u_n^{k*}\left(e^{ik'a} + e^{-ik'a} - 2\right) u_n^{k'} \tag{25}$$
$$= \kappa \sum_{k'} a_{k'}(t)\left(e^{ik'a} + e^{-ik'a} - 2\right)\delta_{kk'} \tag{26}$$
$$= \kappa a_k(t)\left(e^{ika} + e^{-ika} - 2\right) \tag{27}$$
$$= 2\left(\cos(ka) - 1\right)\kappa a_k(t) \tag{28}$$

We have successfully decoupled the differential equations 5, as this result contains only a single term $a_k(t)$. Since $\cos(ka) \le 1$, the coefficient of a_k on the RHS is always negative, so we can write the DE as

$$\ddot{a}_k(t) = 2\frac{\kappa}{m}(\cos(ka) - 1)\, a_k(t) \tag{29}$$
$$= -\omega_k^2 a_k(t) \tag{30}$$

where the oscillator frequency is

$$\omega_k = \sqrt{2\frac{\kappa}{m}(\cos(ka) - 1)} \tag{31}$$
$$= 2\sqrt{\frac{\kappa}{m}}\left|\sin\frac{ka}{2}\right| \tag{32}$$

The differential equation is the standard ODE for a single harmonic oscillator, and has the solutions

$$a_k(t) = \begin{cases} b_k e^{i\omega_k t} \\ b_{-k} e^{-i\omega_k t} \end{cases} \tag{33}$$

where b_k are (possibly complex) constants of integration.

The general solution is a linear combination of these two solutions, but in order to satisfy 19, we must have

$$a_k(t) = b_k e^{i\omega_k t} + b_{-k}^* e^{-i\omega_k t} \tag{34}$$

with

$$b_k^* = b_{-k} \tag{35}$$

Putting all this into 7 and rearranging terms (see Greiner eqs 1.74 - 1.76) gives

$$q_n(t) = \frac{1}{\sqrt{N}} \sum_k \left(b_k e^{-i(\omega_k t - kan)} + b_k^* e^{i(\omega_k t - kan)} \right) \tag{36}$$

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