LINEAR CHAIN OF OSCILLATORS - CLASSICAL TREATMENT, HAMILTONIAN

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

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In the previous post, we saw that for a linear chain of N coupled oscillators we could write the displacement of oscillator n in the chain as

$$q_n(t) = \sum_k \left(b_k e^{-i\omega_k t} u_n^k + b_k^* e^{i\omega_k t} u_n^{k*}\right) \tag{1}$$

$$= \frac{1}{\sqrt{N}} \sum_k \left(b_k e^{-i(\omega_k t - kan)} + b_k^* e^{i(\omega_k t - kan)}\right) \tag{2}$$

where a is the equilibrium separation of two adjacent oscillators, k is given (for periodic boundary conditions) as

$$k = \frac{2\pi}{Na} l \tag{3}$$

where l is an integer in the range

$$-\frac{N}{2} < l \le \frac{N}{2} \tag{4}$$

and

$$\omega_k = 2\sqrt{\frac{\kappa}{m}} \left|\sin\frac{ka}{2}\right| \tag{5}$$

is the frequency of normal mode k. m is the mass at each oscillator and κ is the spring constant.

First, we want an expression for the Hamiltonian, which we can get from 1. The calculation is quite messy, although most of it is spelled out in Greiner's Exercise 1.1 so we don't need to reproduce all that here. The idea is to calculate the kinetic energy T and the potential energy V from 1 and then add them to get $H = T + V$. Classically, the kinetic energy is

$$T = \frac{1}{2} m \sum_{n=1}^{N} \dot{q}_n^2(t) \tag{6}$$

where the time derivative is found from 1:

$$\dot{q}_n(t) = \frac{1}{\sqrt{N}}\sum_k i\omega_k\left(-b_k e^{-i(\omega_k t - kan)} + b_k^* e^{i(\omega_k t - kan)}\right) \tag{7}$$
$$= \sum_k i\omega_k\left(-b_k e^{-i\omega_k t}u_n^k + b_k^* e^{i\omega_k t}u_n^{k*}\right) \tag{8}$$

Inserting the latter form into 6 and multiplying out the terms gives Greiner's equation (1) in Exercise 1.1. This can be simplified by using the completeness relations for the u_n^k:

$$\sum_{n=1}^{N} u_n^{k'*}u_n^k = \delta_{kk'} \tag{9}$$
$$\sum_{k=1}^{N} u_{n'}^{k*}u_n^k = \delta_{nn'} \tag{10}$$

which are derived in equations 1.64 - 1.66. The result is Greiner's equation (3).

The potential energy is given by

$$V = \frac{\kappa}{2}\sum_n\left(q_{n+1} - q_n\right)^2 \tag{11}$$

Again, we need to insert 1 into this expression and multiply out the terms. This results in the very messy eqn (5) in Greiner. We won't derive the entire expression, but it's worth seeing where the first term in his (5) comes from. From 1 we get

$$V = \frac{\kappa}{2}\sum_n\left[\sum_{k'}\left(b_{k'}e^{-i\omega_{k'}t}u_{n+1}^{k'} + b_{k'}^* e^{i\omega_{k'}t}u_{n+1}^{k'*} - b_{k'}e^{-i\omega_{k'}t}u_n^{k'} - b_{k'}^* e^{i\omega_{k'}t}u_n^{k'*}\right)\times\right. \tag{12}$$

$$\left.\sum_k\left(b_k e^{-i\omega_k t}u_{n+1}^k + b_k^* e^{i\omega_k t}u_{n+1}^{k*} - b_{k'}e^{-i\omega_k t}u_n^k - b_k^* e^{i\omega_k t}u_n^{k*}\right)\right] \tag{13}$$

We can now use

$$u_{n+1}^k = e^{ika}u_n^k \tag{14}$$

to get

$$V=\frac{\kappa}{2}\sum_{n}\left[\sum_{k^{\prime}}\left(b_{k^{\prime}}e^{-i\omega_{k^{\prime}}t}e^{ik^{\prime}a}u_{n}^{k^{\prime}}+b_{k^{\prime}}^{*}e^{i\omega_{k^{\prime}}t}e^{-ik^{\prime}a}u_{n}^{k^{\prime}*}-b_{k^{\prime}}e^{-i\omega_{k^{\prime}}t}u_{n}^{k^{\prime}}-b_{k^{\prime}}^{*}e^{i\omega_{k^{\prime}}t}u_{n}^{k^{\prime}*}\right)\times\right. \tag{15}$$

$$\left.\sum_{k}\left(b_{k}e^{-i\omega_{k}t}e^{ika}u_{n}^{k}+b_{k}^{*}e^{i\omega_{k}t}e^{-ika}u_{n}^{k*}-b_{k}e^{-i\omega_{k}t}u_{n}^{k}-b_{k}^{*}e^{i\omega_{k}t}u_{n}^{k*}\right)\right] \tag{16}$$

To get the first line of Greiner's (5), we want the term containing the product $u_n^{k'}u_n^k$ which is formed by multiplying terms in the sum over k' with terms in the sum over k. Specifically, we need to multiply term 1 in the first sum by term 1 in the second, and add term 1 in the first by term 3 in the second, term 3 in the first by term 1 in the second and term 3 in the first by term 3 in the second. This gives the term

$$\frac{\kappa}{2}\sum_{n}\sum_{k,k^{\prime}}b_{k^{\prime}}b_{k}\left(e^{i(k^{\prime}+k)a}-e^{ik^{\prime}a}-e^{ika}+1\right)u_{n}^{k^{\prime}}u_{n}^{k}=\frac{\kappa}{2}\sum_{n}\sum_{k,k^{\prime}}b_{k^{\prime}}b_{k}\left(e^{ik^{\prime}a}-1\right)\left(e^{ika}-1\right)u_{n}^{k^{\prime}}u_{n}^{k} \tag{17}$$

The other 3 lines are derived similarly. Again, we use 9 and 10 to simplify the sums, which leads to Greiner's eqn (6). Then adding $T+V$ and using 5 to convert the complex exponentials in V into ω_k, we find that the Hamiltonian reduces to

$$H=\sum_{k}2m\omega_{k}^{2}b_{k}^{*}b_{k} \tag{18}$$

The Hamiltonian (energy) is independent of time, so energy is conserved.

To find expressions for the coefficients b_k we consider the initial conditions, that is, we consider $q(0)$ and $\dot{q}(0)$ from 1 and 7. Greiner shows that by using the orthogonality relation 10, we get

$$b_{k}+b_{-k}^{*}=\sum_{n}u_{n}^{k*}q_{n}(0) \tag{19}$$

$$-i\omega_{k}\left(b_{k}+b_{-k}^{*}\right)=\sum_{n}u_{n}^{k*}\dot{q}_{n}(0) \tag{20}$$

which can be solved to give

$$b_{k}=\frac{1}{2}\sum_{n}u_{n}^{k*}\left(q_{n}(0)+\frac{i}{\omega_{k}}\dot{q}_{n}(0)\right) \tag{21}$$

Plugging these back into 2 gives the final answer as given in Greiner's eqn 1.80.

$$q_n(t) = \frac{1}{N}\sum_k\sum_{n'}\left[q_{n'}(0)\cos\left(ka\left(n-n'\right)-\omega_k t\right)-\right. \tag{22}$$

$$\left.\frac{1}{\omega_k}\dot{q}_n(0)\sin\left(ka\left(n-n'\right)-\omega_k t\right)\right] \tag{23}$$

Finally, we can calculate the Poisson brackets. To get Greiner's eqn (15), we note that in solving for b_k above, we could have taken $q_n(t)$ and $\dot{q}_n(t)$ at any time t rather than $t=0$. If we do this and work through Greiner's eqns (8) to (11) again to find b_k we end up with his eqn (15):

Choosing $t=0$ just makes the calculation easier.

$$b_k = \frac{1}{2}\sum_n u_n^{k*}e^{i\omega_k t}\left(q_n(t)+\frac{i}{\omega_k}\dot{q}_n(t)\right) \tag{24}$$

$$= \frac{1}{2}\sum_n u_n^{k*}e^{i\omega_k t}\left(q_n(t)+\frac{i}{\omega_k m}p_n(t)\right) \tag{25}$$

The Poisson bracket is

Note that $p_n = m\dot{q}_n$.

$$\left\{b_k, b_{k'}^*\right\} = \sum_n\left(\frac{\partial b_k}{\partial q_n}\frac{\partial b_{k'}^*}{\partial p_n}-\frac{\partial b_k}{\partial p_n}\frac{\partial b_{k'}^*}{\partial q_n}\right) \tag{26}$$

$$= \sum_n\left[u_n^{k*}e^{i\omega_k t}u_n^{k'}e^{-i\omega_{k'}t}\left(-\frac{i}{\omega_{k'}m}\right)-\right. \tag{27}$$

$$\left.\left(\frac{i}{\omega_k m}\right)u_n^{k*}e^{i\omega_k t}u_n^{k'}e^{-i\omega_{k'}t}\right] \tag{28}$$

Using 9 we get Greiner's (17):

$$\left\{b_k, b_{k'}^*\right\} = -\frac{i}{2m\omega_k}\delta_{kk'} \tag{29}$$

The same method gives the other two Poisson brackets:

$$\left\{b_k, b_{k'}\right\} = \left\{b_k^*, b_{k'}^*\right\} = 0 \tag{30}$$

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