LINEAR CHAIN OF OSCILLATORS - QUANTUM TREATMENT

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Reference: W. Greiner & J. Reinhardt, *Field Quantization*, Springer-Verlag (1996), Section 1.5.

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The classical Hamiltonian for a chain of N harmonic oscillators is given by

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

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

To convert this to a quantum version, we replace the position q_n and momentum p_n by their quantum operators and invoke the usual commutation relations

$$[q_n, p_{n'}] = i\hbar\delta_{nn'} \tag{3}$$

$$[q_n, q_{n'}] = [p_n, p_{n'}] = 0 \tag{4}$$

The classical equations for $q_n(t)$ and $p_n(t)$ can be ported over to quantum operators by using normal coordinates, as in the classical case. Greiner gives these as

To save typing, I'll omit the hats over operators in this post. Thus q_n is written as $\hat{q}_n$ in Greiner, and so on.

$$q_n(t) = \sum_k \left(b_k(t)\,u_n^k + b_k^\dagger(t)\,u_n^{k*}\right) \tag{5}$$

$$p_n(t) = -im\sum_k \omega_k\left(b_k(t)\,u_n^k - b_k^\dagger(t)\,u_n^{k*}\right) \tag{6}$$

If you're comparing these equations to the classical ones (eqs 1.74 and 1.77) note that in the classical equations, the coefficients b_k did not depend on time; rather the time dependence was factored out into the $e^{\pm i\omega_k t}$ term. In the quantum case, the operators b_k *do* depend on time, so the $e^{\pm i\omega_k t}$ is assumed to be incorporated into the $b_k(t)$. Also note that in the quantum version, $b_k(t)$ is an operator (so written in full, it would have a hat on it: $\hat{b}_k(t)$).

Note that the $q_n(t)$ and $p_n(t)$ operators as defined in 5 and 6 are hermitian as they must be in order to be observable quantities. For example

$$q_n^\dagger(t) = \sum_k \left(b_k(t)\,u_n^k + b_k^\dagger(t)\,u_n^{k*}\right)^\dagger \tag{7}$$

$$= \sum_k \left(b_k^\dagger(t)\,u_n^{k*} + \left(b_k^\dagger\right)^\dagger(t)\left(u_n^{k*}\right)^*\right) \tag{8}$$

$$= \sum_k \left(b_k^\dagger(t)\,u_n^{k*} + b_k(t)\,u_n^k\right) \tag{9}$$

$$= q_n(t) \tag{10}$$

Note also that b_k is not necessarily hermitian.

The steps followed to derive the classical b_k coefficients also work here, although again remember that the quantum b_ks are time-dependent. The lack of the $e^{\pm i\omega_k t}$ term in 5 and 6 accounts for its absence in Greiner's eqn 1.85:

$$b_k(t) = \frac{1}{2}\sum_n u_n^{k*}\left(q_n(t) + \frac{i}{\omega_k m}p_n(t)\right) \tag{11}$$

Greiner now states that we can determine $b_k(t)$ in terms of $b_k(0)$ by using the relation

$$i\hbar\frac{db_k}{dt} = [b_k, H] \tag{12}$$

We can supposedly evaluate the commutator on the RHS by substituting 2 and 11 into the commutator. This means we need to evaluate the commutator

$$[b_k, H] = \left[\frac{1}{2}\sum_n u_n^{k*}\left(q_n(t) + \frac{i}{\omega_k m}p_n(t)\right), \frac{1}{2m}\sum_{n'} p_{n'}^2 + \frac{\kappa}{2}\sum_{n'}\left(q_{n'+1}(t) - q_{n'}(t)\right)^2\right] \tag{13}$$

Because of the commutation relations 4, we need consider only the two commutators $\left[q_n, p_{n'}^2\right]$ and $\left[p_n, \left(q_{n'+1} - q_{n'}\right)^2\right]$. We can use these relations derived earlier:

$$\left[p_n, q_{n'}^2\right] = -2i\hbar q_n \delta_{nn'} \tag{14}$$

$$\left[q_n, p_{n'}^2\right] = 2i\hbar p_n \delta_{nn'} \tag{15}$$

Applying the second of these, we find that the commutator of the first term from each of b_k and H is:

$$\frac{1}{4m}\sum_{n,n'}u_n^{k*}\left[q_n,p_{n'}^2\right]=\frac{i\hbar}{2m}\sum_{n,n'}u_n^{k*}p_n\delta_{nn'} \tag{16}$$

$$=\frac{i\hbar}{2m}\sum_n u_n^{k*}p_n \tag{17}$$

$$=\hbar\omega_k\frac{i}{2\omega_k m}\sum_n u_n^{k*}p_n \tag{18}$$

This matches the second term in 11.

The other commutator poses a bit of a problem. If we could say that

$$\left[p_n,(q_{n'+1}-q_{n'})^2\right]=\left[p_n,q_{n'}^2\right] \tag{19}$$

we would then have for the commutator of the second term from each of b_k and H:

$$\frac{\kappa i}{4\omega_k m}\left[p_n,(q_{n'+1}-q_{n'})^2\right]=\frac{\kappa i}{4\omega_k m}(-2i\hbar)q_n\delta_{nn'} \tag{20}$$

$$=\frac{\hbar\kappa}{\omega_k m}q_n\delta_{nn'} \tag{21}$$

Using the standard relation between the spring constant κ and the mass and frequency:

$$\omega_k=\sqrt{\frac{\kappa}{m}} \tag{22}$$

we get

$$\frac{\kappa i}{4\omega_k m}\left[p_n,(q_{n'+1}-q_{n'})^2\right]=\hbar\omega_k q_n \tag{23}$$

Inserting this into 13 gives

$$[b_k,H]=\frac{\hbar\omega_k}{2}\sum_n u_n^{k*}\left(q_n(t)+\frac{i}{\omega_k m}p_n(t)\right)=\hbar\omega_k b_k \tag{24}$$

However, it's not entirely clear to me that 19 is valid, since it would appear that if we specify a particular n, then there would be non-zero terms in the commutator from $q_{n'+1}$ when $n'+1=n$ and from $q_{n'}$ when $n'=n$. Comments welcome.

In any case, the equation 11 does allow a straightforward calculation of the commutators for the b_ks, as shown in Greiner's equation 1.88a-b.

$$\left[b_k, b_{k'}^\dagger\right] = \frac{\hbar}{2m\omega_k}\delta_{kk'} \tag{25}$$

$$\left[b_k, b_{k'}\right] = \left[b_k^\dagger, b_{k'}^\dagger\right] = 0 \tag{26}$$

From 5 and the fact that the normal coordinates u_n^k are dimensionless, we see that the operators b_k have the same dimensions as the position coordinates q_n, so they have the dimension of length. To introduce dimensionless operators, we define

$$c_k \equiv \sqrt{\frac{2m\omega_k}{\hbar}} b_k \tag{27}$$

which means we can write the position and momentum as

$$q_n(t) = \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} \left(c_k(t)\,u_n^k + c_k^\dagger(t)\,u_n^{k*}\right) \tag{28}$$

$$p_n(t) = -i\sum_k \sqrt{\frac{\hbar m\omega_k}{2}} \left(c_k(t)\,u_n^k - c_k^\dagger(t)\,u_n^{k*}\right) \tag{29}$$

The commutation relations are then

$$\left[c_k, c_{k'}^\dagger\right] = \delta_{kk'} \tag{30}$$

$$\left[c_k, c_{k'}\right] = \left[c_k^\dagger, c_{k'}^\dagger\right] = 0 \tag{31}$$

To get the Hamiltonian in terms of these dimensionless operators, we can follow through the derivation of H that we did for the classical case. The crucial difference in the derivation of the quantum result is that c_k and $c_k^\dagger$ are now operators that don't commute, so when we plug 28 and 29 into 2, we must remember to maintain the order of the operators. Apart from that, the derivation goes the same as before, and we get

$$H = \sum_k \hbar\omega_k \left(c_k^\dagger c_k + \frac{1}{2}\right) \tag{32}$$

This is just what we'd expect for the energy of a collection of uncoupled harmonic oscillators. One thing that isn't entirely clear to me, however, is that Greiner seems to be assuming that all the frequencies ω_k are equal (to $\sqrt{\kappa/m}$) so I'm not sure why there is a subscript k on ω_k.

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