Ring of N Classical or Quantum Harmonic Oscillators

1 The Classsical Oscillator

The equation of motion for the nth oscillator in a ring of N coupled classical harmonic oscillators is given by

$$\ddot{q}_n = \frac{k}{m}(q_{n+1} + q_{n-1} - 2q_n) \tag{1}$$

where $n = n + N$ and a dot denotes differentiation with respect to time. This can be written more compactly as

$$\ddot{\mathbf{q}} = -K\mathbf{q} \tag{2}$$

where $\mathbf{q}$ is a vector of displacements of individual oscillators at time t and K is the matrix with components

$$K_{ij} = \frac{k}{m}(2\delta_{ij} - \delta_{i+1,j} - \delta_{i-1,j}) \tag{3}$$

with δ_{ij} the Kronecker delta. To solve this equation, we can use the method of normal modes, where we assume every oscillator oscillates with the same frequency ω, i.e.

$$\mathbf{q}(t) = \mathbf{A}\cos(\omega t - \delta) \tag{4}$$

where δ is a phase. Hence,

$$\omega^2\mathbf{A} = K\mathbf{A} \quad \Rightarrow \quad \det\left(K - \omega^2\mathbb{1}\right) = 0 \tag{5}$$

where $\mathbb{1}$ is the $N \times N$ identity matrix. So, the normal mode frequencies will be given by the eigenvalues of the matrix K, and $\mathbf{A}$ will be given by the eigenvectors. Since this specifies a basis of solutions, a general solution will be of the form

$$\mathbf{q}(t) = \sum_i a_i\mathbf{A}_i\cos(\omega_i t - \delta) = \sum_i \left(\alpha_i\mathbf{A}_i\cos(\omega_i t) + \beta_i\mathbf{A}_i\sin(\omega_i t)\right) \tag{6}$$

where i runs over the number of normal modes and α_i and β_i are constants. Thus, our differential equation turns into a set of algebraic equations which we can solve given initial conditions.

2 The Quantum Oscillator

2.1 Discrete Case

Start with a ring of N identical, simple (classical) harmonic oscillators with equilibrium separation ϵ. The Hamiltonian is given by

$$H = \sum_{n=0}^{N-1}\left(\frac{p_n^2}{2m} + \frac{\alpha}{2}\left(q_{n+1} - q_n\right)^2\right) \tag{7}$$

The periodicity constraint implies $n = n + N$. To solve, take positions and momenta to Fourier space

$$p_n = \frac{1}{\sqrt{N}}\sum_{j=-N/2}^{N/2} e^{-ik_j x_n}\tilde{p}_j, \qquad q_n = \frac{1}{\sqrt{N}}\sum_{j=-N/2}^{N/2} e^{-ik_j x_n}\tilde{q}_j \tag{8}$$

where

$$k_j \equiv \frac{2\pi j}{N\epsilon}, \quad x_n \equiv n\epsilon \tag{9}$$

First, looking at the kinetic energy term,

$$T = \frac{1}{2mN} \sum_{n=0}^{N-1} \sum_{j=-N/2}^{N/2} \sum_{i=-N/2}^{N/2} e^{-ix_n(k_j+k_i)} \tilde{p}_j \tilde{p}_i = \sum_{-N/2}^{N/2} \frac{|\tilde{p}_j|^2}{2m} \tag{10}$$

where the orthonormality of the basis functions as well as $p_n \in \mathbb{R}$ were used

$$\frac{1}{N} \sum_{n=0}^{N-1} e^{-ix_n(k_j-k_i)} = \delta_{ij}, \qquad \tilde{p}_{-j} = \tilde{p}_j^* \text{ for } p_n \in \mathbb{R} \tag{11}$$

Now, the potential energy term,

$$\begin{aligned} V = \frac{\alpha}{2N} \sum_{n=0}^{N-1} \sum_{j=-N/2}^{N/2} \sum_{i=-N/2}^{N/2} \Big[& e^{-ix_{n+1}(k_i+k_j)} \tilde{q}_i \tilde{q}_j + e^{-ix_n(k_i+k_j)} \tilde{q}_i \tilde{q}_j \\ & - \left(e^{-i(k_i x_n + k_j x_{n+1})} + e^{-i(k_j x_n + k_i x_{n+1})} \right) \tilde{q}_i \tilde{q}_j \Big] \end{aligned} \tag{12}$$

Here, the symmetry of the sums over i and j are used to re-index the term in parenthesis. Focusing on this term, we use the periodicity of n to re-index the x_n's using $x_{n\pm1} = (n \pm 1)\epsilon$

$$\sum_{n=0}^{N-1} \left(e^{-i(k_i x_n + k_j x_{n+1})} + e^{-i(k_j x_{n-1} + k_i x_n)} \right) = \sum_{n=0}^{N-1} e^{-ix_n(k_i+k_j)} \left(e^{-ik_j\epsilon} + e^{ik_j\epsilon} \right) = 2N\cos(k_j\epsilon)\delta_{i,-j} \tag{13}$$

which gives

$$V = \frac{\alpha}{2} \sum_{j=-N/2}^{N/2} 2\big(1-\cos(k_j\epsilon)\big)|\tilde{q}_j|^2 \equiv \sum_{j=-N/2}^{N/2} \frac{m\omega_j^2}{2} |\tilde{q}_j|^2 \quad \text{where} \quad \omega_j^2 \equiv \frac{2\alpha}{m}\big(1-\cos(k_j\epsilon)\big) \tag{14}$$

Now, we just quantize by upgrading $\tilde{q}_j \to \tilde{Q}_j$ and $\tilde{p}_j \to \tilde{P}_j$ where $\tilde{Q}_j$ and $\tilde{P}_j$ are Hermitian operators satisfying

$$\big[\tilde{Q}_j, \tilde{P}_{j'}\big] = i\delta_{jj'} \tag{15}$$

We then define creation and annihilation operators

$$\tilde{Q}_j = \frac{1}{\sqrt{2m\omega_j}} \big(\tilde{a}_j^\dagger + \tilde{a}_j\big), \quad \tilde{P}_j = i\sqrt{\frac{m\omega_j}{2}} \big(\tilde{a}_j^\dagger - \tilde{a}_j\big) \tag{16}$$

which satisfy

$$\big[\tilde{a}_j, \tilde{a}_{j'}^\dagger\big] = \delta_{jj'}, \quad \big[\tilde{a}_j, \tilde{a}_{j'}\big] = \big[\tilde{a}_j^\dagger, \tilde{a}_{j'}^\dagger\big] = 0 \tag{17}$$

giving the Hamiltonian of N QHO's

$$H = \sum_{j=-N/2}^{N/2} \omega_j \left(\tilde{a}_j^\dagger \tilde{a}_j + \frac{1}{2} \right) \tag{18}$$

This Hamiltonian acts on the Fock space of states

$$|\psi\rangle = \bigotimes_{j=-N/2}^{N/2} |n_j\rangle \equiv \big|n_{(-N/2)}, n_{(-(N-1)/2)}, ..., n_{N/2}\big\rangle \tag{19}$$

where n_j is the number of quanta of energy in mode j. Now, we want to find the creation/annihilation operators in position space. We may guess they take the form

$$a_n = \frac{1}{\sqrt{N}} \sum_{j=-N/2}^{N/2} e^{-ik_j x_n} \tilde{a}_j, \quad a_n^\dagger = \frac{1}{\sqrt{N}} \sum_{j=-N/2}^{N/2} e^{ik_j x_n} \tilde{a}_j^\dagger \tag{20}$$

We check that these do indeed satisfy the correct commutation relations for creation/annihilation operators

$$\left[a_n, a_{n'}^\dagger\right] = \frac{1}{N} \sum_{j=-N/2}^{N/2} \sum_{i=-N/2}^{N/2} e^{-i(k_j x_n - k_i x_{n'})} \left[\tilde{a}_j, \tilde{a}_i^\dagger\right] = \frac{1}{N} \sum_{j=-N/2}^{N/2} e^{-ik_j(x_n - x_{n'})} = \delta_{nn'} \tag{21}$$

with all other commutation relations vanishing as expected. With this, we place a single quanta of energy in the n^{th} position by acting on the vacuum with $a_n^\dagger$

$$|\psi_n\rangle = a_n^\dagger |0\rangle = \frac{1}{\sqrt{N}} \sum_{j=-N/2}^{N/2} e^{ik_j x_n} \tilde{a}_j^\dagger |0\rangle = \frac{1}{\sqrt{N}} \sum_{j=-N/2}^{N/2} e^{ik_j x_n} |j\rangle \tag{22}$$

where $|j\rangle \equiv |0, 0, \ldots, 1, \ldots, 0, 0\rangle$ with a 1 in the j^{th} mode. Now, we want to time-evolve this state with the Hamiltonian and find the amplitude for the particle to be at some different position, m. Neglecting the zero-point energy, the energy of the single-quanta state j is given by

$$H |j\rangle = E_j |j\rangle = \omega_j |j\rangle \tag{23}$$

So, our desired amplitude is given by

$$\langle\psi_m| e^{-iHt} |\psi_n\rangle = \frac{1}{N} \sum_{j=-N/2}^{N/2} e^{ik_j(x_n - x_m)} e^{-i\omega_j t} = \frac{1}{N} \sum_{j=-N/2}^{N/2} e^{i\frac{2\pi j}{N}(n-m)} e^{-i\omega_j t} \tag{24}$$

2.2 Continuum Case

Let's study this more explicitly in the continuum case. When we take $\epsilon \to 0$, we write our Hamiltonian as

$$H = \sum_{n=0}^{N-1} \epsilon \left(\frac{p_n^2}{2m\epsilon} + \frac{\alpha\epsilon}{2} \left(\frac{q_{n+1} - q_n}{\epsilon} \right)^2 \right) \tag{25}$$

Now, when we take the limit, our position and momentum variables become functions of x and t, the term in parenthesis becomes a derivative, and the sum is upgraded to an integral over position. Defining new fields and constants

$$\pi(x,t) = \epsilon p(x,t), \quad \phi(x,t) = q(x,t), \quad \rho = \frac{m}{\epsilon}, \quad \beta = \epsilon\alpha \tag{26}$$

giving the Hamiltonian

$$H = \int_0^L dx \left(\frac{\pi(x)^2}{2\rho} + \frac{\beta}{2} \left(\frac{\partial\phi}{\partial x} \right)^2 \right) \tag{27}$$

Again, transforming to Fourier space (keeping in mind that we must use a discrete Fourier transform due to the periodic boundary conditions)

$$\pi(x,t) = \frac{1}{\sqrt{L}} \sum_{j=-\infty}^{\infty} e^{-ik_j x} \tilde{\pi}(k_j, t), \quad \phi(x,t) = \frac{1}{\sqrt{L}} \sum_{j=-\infty}^{\infty} e^{-ik_j x} \tilde{\phi}(k_j, t) \tag{28}$$

where now, the momenta are defined by

$$k_j \equiv \frac{2\pi j}{L} \tag{29}$$

since we take $N \to \infty$ and $\epsilon \to 0$ while keeping L fixed.

Plugging these into H,

$$\begin{aligned} H =& \frac{1}{L}\int_0^L dx \sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty} e^{-ix(k_j+k_{j'})}\left[\frac{\tilde{\pi}(k_j)\tilde{\pi}(k_{j'})}{2\rho} + \frac{\beta}{2}(-ik_j)(-ik_{j'})\tilde{\phi}(k_j)\tilde{\phi}(k_{j'})\right] \\ =& \sum_{j=-\infty}^{\infty}\left[\frac{|\tilde{\pi}(k_j)|^2}{2\rho} + \frac{\beta k_j^2}{2}|\tilde{\phi}(k_j)|^2\right] \equiv \sum_{k_j=-\infty}^{\infty}\left[\frac{|\tilde{\pi}(k_j)|^2}{2\rho} + \frac{\rho\omega(k_j)^2}{2}|\tilde{\phi}(k_j)|^2\right] \end{aligned} \tag{30}$$

where

$$\omega(k_j)^2 = \frac{\beta}{\rho}k_j^2 \equiv c_s^2 k_j^2 \tag{31}$$

We again play the same game with upgrading position/momentum variables to operators and defining position and momentum space creation/annihilation operators such that

$$a(x) = \frac{1}{\sqrt{L}}\sum_{j=-\infty}^{\infty} e^{-ik_j x}\tilde{a}(k_j), \quad a(x)^\dagger = \frac{1}{\sqrt{L}}\sum_{j=-\infty}^{\infty} e^{ik_j x}\tilde{a}(k_j)^\dagger \tag{32}$$

It is easy to see that these satisfy the correct commutation relations, as before.

Again, we create a single-quanta state at point x and want to find the amplitude of finding it at point y after time t. This amplitude is now given by

$$\langle\psi(y)|\, e^{-iHt}\,|\psi(x)\rangle = \frac{1}{L}\sum_{j=-\infty}^{\infty} e^{ik_j(x-y)}e^{-i\omega(k_j)t} = \frac{1}{L}\sum_{j=-\infty}^{\infty} e^{ik_j(x-y)}e^{-i|k_j|c_s t} \tag{33}$$

This sum can be evaluated exactly to find

$$K(x,y;t) = \langle\psi(y)|\, e^{-iHt}\,|\psi(x)\rangle = \frac{i}{L}\frac{\sin(2\pi c_s t/L)}{\cos(2\pi c_s t/L) - \cos(2\pi(x-y)/L)} \tag{34}$$

Note that as we take $L \to \infty$, this reduces to

$$K(x,y;t) = \frac{2ic_s t}{(x-y)^2 - c_s^2 t^2} \tag{35}$$

which is exactly what we expect from the Fourier transform of $\exp(-i|k|c_s t)$.

A comment is in order about how to interpret this. If we take $K(x,y;t)$ at face value, then it gives some distribution around the ring which is non-zero everywhere. However, we need to be careful. Remember that this is an amplitude, meaning that when we take the magnitude squared, we should find a probability, which should never exceed one. Looking at our expression for the amplitude, we see that, not only will the probability be greater than one in several places, but it in fact diverges at the two poles, $x - y = \pm c_s t$! To get this to behave like a probability, we should normalize our states so that it is bounded between zero and one, and so that the total probability over the whole ring is one. To do this, we essentially will need to divide everything by an infinite factor (because of the divergences at the poles), which will kill off any finite contribution. This leaves only the contributions from the two poles, which, of course, describes a point particle travelling around the ring at the speed of sound c_s (a phonon). It seems that a theory of quantum fields describes the movement of particles!