The One-Dimensional Harmonic Oscillator

Quantum Mechanics, 2\textsuperscript{nd} Edition, Cohen-Tannoudji
Chapter V
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Outline

The Classical Harmonic Oscillator

The Quantum Harmonic Oscillator

Systems of Two Coupled Oscillators

Systems of Infinitely Coupled Oscillators: Phonons
The Classical Harmonic Oscillator

The simplest case is a particle of mass \( m \) moving in a potential given by \( V(x) \):

\[
V(x) = \frac{1}{2} k x^2 \quad F_x = -\frac{dV}{dx} = -kx \quad m \frac{d^2x}{dt^2} = -\frac{dV}{dx} = -kx
\]

Experiencing a restoring force \( F_x \)

Solutions to the equation of motion take the form:

\[
x = x_m \cos(\omega t - \varphi) \quad \omega = \sqrt{\frac{k}{m}} \quad x_m \text{ and } \varphi \text{ are integration constants depending on initial conditions}
\]

The kinetic and total energy follow:

\[
T = \frac{1}{2} m \left(\frac{dx}{dt}\right)^2 = \frac{p^2}{2m} \quad E = T + V = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2
\]
A comment on where we can find harmonic oscillators...

For any arbitrary potential $V(x)$, we can write a Taylor expansion as:

$$V(x) = a + b(x - x_0)^2 + c(x - x_0)^3 + \ldots$$

$$F_x = -\frac{dV}{dx} = -2b(x - x_0) - 3c(x - x_0)^2 + \ldots$$

If the displacement is small such that higher order terms can be neglected:

$$m \frac{d^2x}{dt^2} \simeq -2b(x - x_0)$$

$$\omega = \sqrt{\frac{2b}{m}} = \sqrt{\frac{1}{m} \left( \frac{d^2V}{dx^2} \right)_{x = x_0}}$$

...we can treat our arbitrary potential well as a harmonic oscillator.
A comment on where we can find harmonic oscillators...

From Boyd, Nonlinear Optics:

Electrons in noncentrosymmetric media see anharmonic potential wells...

\[
\ddot{x} + 2\gamma \dot{x} + \omega_0^2 x + a\dot{x}^2 = -e\tilde{E}(t)/m.
\]

\[
\tilde{F}_{\text{restoring}} = -m\omega_0^2 \dot{x} - ma\dot{x}^2
\]

where \( a \) is a measure of the nonlinearity.

\[
U(\tilde{x}) = -\int \tilde{F}_{\text{restoring}} d\tilde{x} = \frac{1}{2}m\omega_0^2 \tilde{x}^2 + \frac{1}{3}ma\tilde{x}^3.
\]

For weak electric fields resulting in small electron displacements, linear optical properties are sufficient for describing a material response.

The bottom of this well can be approximated as harmonic.
The Quantum Harmonic Oscillator

\[ E = T + V = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \]

We can simply replace classical position and momentum with quantum observables:

\[ H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \quad [X, P] = i\hbar \]

\[ H | \varphi \rangle = E | \varphi \rangle \]

\[ \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right] \varphi(x) = E \varphi(x) \]

We will start to introduce new operators for convenience:

\[ \hat{X} = \sqrt{\frac{m\omega}{\hbar}} X \quad [\hat{X}, \hat{P}] = i \]

\[ \hat{P} = \frac{1}{\sqrt{m\hbar\omega}} P \]

\[ H = \hbar \omega \hat{H} \quad \hat{H} = \frac{1}{2} (\hat{X}^2 + \hat{P}^2) \]

\[ \hat{H} | \varphi_v \rangle = \varepsilon_v | \varphi_v \rangle \]
Introducing New Operators

We’d like to write this using terms linear in $X^\dagger$ and $P^\dagger$ but that’s not so easy...

Since they do not commute, we cannot treat them as simple variables:

\[
\hat{X}^2 + \hat{P}^2 \neq (\hat{X} - i\hat{P})(\hat{X} + i\hat{P})
\]

\[
a = \frac{1}{\sqrt{2}} (\hat{X} + i\hat{P}) \quad \hat{X} = \frac{1}{\sqrt{2}} (a^\dagger + a)
\]

\[
a^\dagger = \frac{1}{\sqrt{2}} (\hat{X} - i\hat{P}) \quad \hat{P} = \frac{i}{\sqrt{2}} (a^\dagger - a)
\]

\[
[a, a^\dagger] = \frac{1}{2} [\hat{X} + i\hat{P}, \hat{X} - i\hat{P}]
\]

\[
= \frac{i}{2} [\hat{P}, \hat{X}] - \frac{i}{2} [\hat{X}, \hat{P}]
\]

\[
= 1
\]
Introducing New Operators

\[ a = \frac{1}{\sqrt{2}} (\hat{X} + i\hat{P}) \quad a^*a = \frac{1}{2} (\hat{X} - i\hat{P})(\hat{X} + i\hat{P}) \]
\[ a^* = \frac{1}{\sqrt{2}} (\hat{X} - i\hat{P}) \]
\[ = \frac{1}{2} (\hat{X}^2 + \hat{P}^2 + i\hat{X}\hat{P} - i\hat{P}\hat{X}) \]
\[ = \frac{1}{2} (\hat{X}^2 + \hat{P}^2 - 1) \]
\[ \hat{H} = aa^* - \frac{1}{2} \]

We are going to try to solve the Harmonic oscillator using \( a, a^* \), and \( N \):

\[ N = a^*a \quad N^* = a^*(a^*)^* = a^*a = N \]
\[ N \mid \varphi_i^* \rangle = \nu \mid \varphi_i^* \rangle \]
\[ [N, a] = [a^*a, a] = a^*[a, a] + [a^*, a]a = -a \]
\[ [N, a^*] = [a^*a, a^*] = a^*[a, a^*] + [a^*, a^*]a = a^* \]
\[ H \mid \varphi_i^* \rangle = (\nu + 1/2)\hbar\omega \mid \varphi_i^* \rangle \]
Introducing New Operators

\[ a = \frac{1}{\sqrt{2}} (\hat{X} + i\hat{P}) \quad \quad [N, a] = -a \]
\[ a^\dagger = \frac{1}{\sqrt{2}} (\hat{X} - i\hat{P}) \quad \quad [N, a^\dagger] = a^\dagger \]

A reminder that \( N \) and \( H \) share eigenvectors (eigenstates).

\[
\begin{align*}
[N, a] | \phi_v^i \rangle &= -a | \phi_v^i \rangle \\
Na | \phi_v^i \rangle &= aN | \phi_v^i \rangle - a | \phi_v^i \rangle \\
&= a \nu | \phi_v^i \rangle - a | \phi_v^i \rangle \\
N[a | \phi_v^i \rangle] &= (\nu - 1) [a | \phi_v^i \rangle]
\end{align*}
\]

\[
\begin{align*}
[N, a^\dagger] | \phi_v^i \rangle &= a^\dagger | \phi_v^i \rangle \\
Na^\dagger | \phi_v^i \rangle &= a^\dagger N | \phi_v^i \rangle + a^\dagger | \phi_v^i \rangle \\
&= (\nu + 1) a^\dagger | \phi_v^i \rangle
\end{align*}
\]

\( a \) and \( a^\dagger \) are commonly named creation and annihilation/destruction operators, or ladder operators because of this property.
The Spectrum of $N$

The spectrum of $N$ must be positive or zero.

\[ v - n \quad v - n + 1 \quad v - 1 \quad v \]

\[ a^* | \varphi_i^i \rangle \quad a^{* -1} | \varphi_i^i \rangle \quad a | \varphi_i^i \rangle \quad | \varphi_i^i \rangle \]

\[ \| a | \varphi_i^i \rangle \|^2 = \langle \varphi_i^i | a^* a | \varphi_i^i \rangle \geq 0 \]

\[ \langle \varphi_i^i | a^* a | \varphi_i^i \rangle = \langle \varphi_i^i | N | \varphi_i^i \rangle = v \langle \varphi_i^i | \varphi_i^i \rangle \]

\[ v \geq 0 \]

Eigenvalues of $N$ must be positive or zero.
The Spectrum of $N$

For an arbitrary, nonintegral eigenvalue $v$:

$$n < v < n + 1 \quad |\varphi_v^i\rangle, \quad a |\varphi_v^i\rangle \quad ... \quad a^n |\varphi_v^i\rangle$$

If $|\varphi_v^i\rangle$ is non-zero, then $a |\varphi_v^i\rangle$ is non-zero with eigenvalue $v - 1$. Any $a^p |\varphi_v^i\rangle$ is obtained by the action of $a$ on the state with strictly positive eigenvalue $v - p + 1$, since $p \leq n$ and $v > n$.

If we act again with $a$ on $a^n |\varphi_v^i\rangle$, we must get a non-zero vector. But, $a^{n+1} |\varphi_v^i\rangle$ has eigenvalue $v - n - 1$ which is strictly negative. Since it is impossible to construct a non-zero eigenvector of $N$ with a strictly negative eigenvalue, $v$ must be an integer.

$$v = n$$

Then $a^n |\varphi_v^i\rangle$ has eigenvalue 0 and $a^{n+1} |\varphi_v^i\rangle = 0$.

$v$ must be a non-negative integer.
The Spectrum of $N$

We have concluded the energies of the harmonic oscillator are quantized purely through the properties of $a$ and $a^\dagger$. 

$$H | \phi_v^i \rangle = (v + 1/2)\hbar\omega | \phi_v^i \rangle$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$
Eigenstates of the Hamiltonian

Let’s understand the ground state...

\[ a \, \phi_0 \neq 0 \]

\[
\frac{1}{\sqrt{2}} \left[ \sqrt{\frac{m\omega}{\hbar}} X + \frac{i}{\sqrt{m\hbar \omega}} P \right] \phi_0 = 0
\]

Written analytically:

\[
\left( \frac{m \omega}{\hbar} x + \frac{d}{dx} \right) \phi_0(x) = 0
\]

\[ \phi_0(x) = c \, e^{-\frac{1}{2} \frac{m \omega}{\hbar} x^2} \]

\[ \phi_0(x) = \langle x | \phi_0 \rangle = \left( \frac{m \omega}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{1}{2} \frac{m \omega}{\hbar} x^2} \]

Now for higher level states:

\[ | \phi_1 \rangle = c_1 a^\dagger | \phi_0 \rangle \]

\[
\langle \phi_1 | \phi_1 \rangle = |c_1|^2 \langle \phi_0 | a a^\dagger | \phi_0 \rangle
\]

\[
= |c_1|^2 \langle \phi_0 | (a^\dagger a + 1) | \phi_0 \rangle
\]

\[
\langle \phi_1 | \phi_1 \rangle = |c_1|^2 = 1
\]

\[ | \phi_2 \rangle = c_2 a^\dagger | \phi_1 \rangle \]

\[
\langle \phi_2 | \phi_2 \rangle = |c_2|^2 \langle \phi_1 | a a^\dagger | \phi_1 \rangle
\]

\[
= |c_2|^2 \langle \phi_1 | (a^\dagger a + 1) | \phi_1 \rangle
\]

\[ = 2 |c_2|^2 = 1 \]
Eigenstates of the Hamiltonian

Generally:

\[ |\varphi_1\rangle = c_1 a^\dagger |\varphi_0\rangle \]

\[
\langle \varphi_1 | \varphi_1 \rangle = |c_1|^2 \langle \varphi_0 | a a^\dagger | \varphi_0 \rangle
= |c_1|^2 \langle \varphi_0 | (a^\dagger a + 1) | \varphi_0 \rangle
= |c_1|^2 = 1
\]

\[ |\varphi_2\rangle = c_2 a^\dagger |\varphi_1\rangle \]

\[
\langle \varphi_2 | \varphi_2 \rangle = |c_2|^2 \langle \varphi_1 | a a^\dagger | \varphi_1 \rangle
= |c_2|^2 \langle \varphi_1 | (a^\dagger a + 1) | \varphi_1 \rangle
= 2 |c_2|^2 = 1
\]

\[
\langle \varphi_n | \varphi_n \rangle = |c_n|^2 \langle \varphi_{n-1} | a a^\dagger | \varphi_{n-1} \rangle
= n |c_n|^2 = 1
\]

\[ |\varphi_n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |\varphi_0\rangle \]

\[ a^\dagger = \frac{1}{\sqrt{2}} \left[ \sqrt{\frac{\hbar}{m\omega}} x - \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx} \right] \]

\[ \varphi_n(x) = \langle x | \varphi_n \rangle = \frac{1}{\sqrt{n!}} \langle x | (a^\dagger)^n | \varphi_0 \rangle \]

\[ = \frac{1}{\sqrt{n!} \sqrt{2^n}} \left[ \sqrt{\frac{m\omega}{\hbar}} x - \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx} \right]^n \varphi_0(x) \]
Eigenstates of the Hamiltonian

\[ \varphi_n(x) = \left[ \frac{1}{2^n n!} \left( \frac{\hbar}{m\omega} \right)^n \right]^{1/2} \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \left[ m\omega \frac{x}{\hbar} - \frac{d}{dx} \right]^n e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} \]

These are known as Hermite polynomials.

**Figure 4**
Wave functions associated with the first three levels of a harmonic oscillator.

**Figure 5**
Probability densities associated with the first three levels of a harmonic oscillator.
Normal Modes of Two Coupled Oscillators

The simple (but trivial) case of two uncoupled oscillators:

\[ U_0(x_1, x_2) = \frac{1}{2} m\omega^2(x_1 - a)^2 + \frac{1}{2} m\omega^2(x_2 + a)^2 \]

\[
\begin{aligned}
F_1 &= -\frac{\partial}{\partial x_1} U_0(x_1, x_2) = -m\omega^2(x_1 - a) \\
F_2 &= -\frac{\partial}{\partial x_2} U_0(x_1, x_2) = -m\omega^2(x_2 + a)
\end{aligned}
\]

\[
\begin{aligned}
m\frac{d^2}{dt^2} x_1(t) &= -m\omega^2 (x_1 - a) \\
m\frac{d^2}{dt^2} x_2(t) &= -m\omega^2 (x_2 + a)
\end{aligned}
\]

They behave as independent particles with the solutions we have just examined.

Now let’s provide a coupling potential:

\[ U(x_1, x_2) = U_0(x_1, x_2) + V(x_1, x_2) \]

\[ V(x_1, x_2) = \lambda m\omega^2(x_1 - x_2)^2 \]

\[
\begin{aligned}
F'_1 &= -\frac{\partial}{\partial x_1} V(x_1, x_2) = 2\lambda m\omega^2(x_2 - x_1) \\
F'_2 &= -\frac{\partial}{\partial x_2} V(x_1, x_2) = 2\lambda m\omega^2(x_1 - x_2)
\end{aligned}
\]

We must add the forces \( F'_1 \) and \( F'_2 \) to \( F_1 \) and \( F_2 \).
Classical Treatment of Coupled Oscillators

The equation of motion becomes:

\[
\begin{align*}
\frac{m}{dt^2} x_1(t) &= -m\omega^2 (x_1 - a) \\
\frac{m}{dt^2} x_2(t) &= -m\omega^2 (x_2 + a)
\end{align*}
\]

Can solve coupled differential equations by diagonalizing the matrix of coefficients:

\[
K = -m\omega^2 \begin{pmatrix} 1 + 2\lambda & -2\lambda \\ -2\lambda & 1 + 2\lambda \end{pmatrix}
\]

\[
x_G(t) = \frac{1}{2} [x_1(t) + x_2(t)] \\
x_R(t) = x_1(t) - x_2(t)
\]

\[
\begin{align*}
x_1(t) &= x_G(t) + \frac{1}{2} x_R(t) \\
x_2(t) &= x_G(t) - \frac{1}{2} x_R(t)
\end{align*}
\]
Classical Treatment of Coupled Oscillators

\[ \mathcal{H}(x_1, x_2, p_1, p_2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + U_0(x_1, x_2) + V(x_1, x_2) \]

\[
\begin{align*}
\begin{cases}
  p_G(t) = p_1(t) + p_2(t) \\
  p_R(t) = \frac{1}{2} [ p_1(t) - p_2(t) ]
\end{cases}
\end{align*}
\]

\[
\begin{align*}
\begin{cases}
  \mu_G = 2m \\
  \mu_R = \frac{m}{2}
\end{cases}
\end{align*}
\]

\[ \mathcal{H} = \frac{p_G^2}{2\mu_G} + \frac{1}{2} \mu_G \omega_G^2 x_G^2 + \frac{p_R^2}{2\mu_R} + \frac{1}{2} \mu_R \omega_R^2 \left( x_R - \frac{2a}{1 + 4\lambda} \right)^2 \\
+ m\omega^2 a^2 \frac{4\lambda}{1 + 4\lambda} \]

By a change in the energy origin, the last term can be removed.

There is no coupling remaining in the Hamiltonian, indicating the modes we solved for are indeed independent.
Quantum Treatment of Coupled Oscillators

The quantum mechanical perspective starts with a replacement by analogous observables:

\[
x_G(t) = \frac{1}{2} [x_1(t) + x_2(t)]
\]

\[
x_R(t) = x_1(t) - x_2(t)
\]

\[
\begin{align*}
  p_G(t) &= p_1(t) + p_2(t) \\
p_R(t) &= \frac{1}{2} [ p_1(t) - p_2(t) ]
\end{align*}
\]

\[
\begin{align*}
  X_G &= \frac{1}{2} (X_1 + X_2) \\
P_G &= P_1 + P_2
\end{align*}
\]

\[
\begin{align*}
  X_R &= X_1 - X_2 \\
P_R &= \frac{1}{2} (P_1 - P_2)
\end{align*}
\]

\[
\begin{align*}
  [X_G, P_G] &= \frac{1}{2} \{ [X_1, P_1] + [X_1, P_2] + [X_2, P_1] + [X_2, P_2] \} \\
  &= \frac{1}{2} \{ i\hbar + i\hbar \} = i\hbar
\end{align*}
\]

\[
\begin{align*}
  [X_G, P_R] &= \frac{1}{4} \{ [X_1, P_1] - [X_1, P_2] + [X_2, P_1] - [X_2, P_2] \} \\
  &= \frac{1}{4} \{ i\hbar - i\hbar \} = 0
\end{align*}
\]

Observables for each particle are independent and commute. The same follows for the modes.

Interestingly enough, the modes also preserve the canonical commutation relation.
Quantum Treatment of Coupled Oscillators

\[ H = T + U \]
\[ T = \frac{1}{2m} \left( P_1^2 + P_2^2 \right) \]
\[ U = \frac{1}{2} m\omega^2 \left[ (X_1 - a)^2 + (X_2 + a)^2 + 2\lambda(X_1 - X_2)^2 \right] \]
\[
\begin{cases}
\mu_G = 2m \\
\mu_R = \frac{m}{2}
\end{cases}
\]
\[ U = \frac{1}{2} \mu_G\omega_G^2 X_G^2 + \frac{1}{2} \mu_R\omega_R^2 \left( X_R - \frac{2a}{1 + 4\lambda} \right)^2 + m\omega^2 a^2 \frac{4\lambda}{1 + 4\lambda} \]

\[ H = H_G + H_R + m\omega^2 a^2 \frac{4\lambda}{1 + 4\lambda} \]
\[
\begin{cases}
H_G = \frac{P_G^2}{2\mu_G} + \frac{1}{2} \mu_G\omega_G^2 X_G^2 \\
H_R = \frac{P_R^2}{2\mu_R} + \frac{1}{2} \mu_R\omega_R^2 \left[ X_R - \frac{2a}{1 + 4\lambda} \right]^2
\end{cases}
\]

By a substitution of the corresponding observables, we can eventually see that the quantum mechanical Hamiltonian is also uncoupled in the system of defined by the modes.
Quantum Treatment of Coupled Oscillators

\[
\begin{align*}
H_G &= \frac{P_G^2}{2\mu_G} + \frac{1}{2} \mu_G \omega_G^2 X_G^2 \\
H_R &= \frac{P_R^2}{2\mu_R} + \frac{1}{2} \mu_R \omega_R^2 \left[ X_R - \frac{2a}{1 + 4\lambda} \right]^2
\end{align*}
\]

\[
| \varphi_{n,p} \rangle = | \varphi_n^G \rangle | \varphi_p^R \rangle = \frac{(a_G^t)^n (a_R^t)^p}{\sqrt{n!} \ p!} | \varphi_{0,0} \rangle \\
E_{n,p} = E_n^G + E_p^R + m\omega^2a^2 \frac{4\lambda}{1 + 4\lambda}
\]

\[
= \left( n + \frac{1}{2} \right) \hbar \omega_G + \left( p + \frac{1}{2} \right) \hbar \omega_R + m\omega^2a^2 \frac{4\lambda}{1 + 4\lambda}
\]

\[
a_G^t | \varphi_{n,p} \rangle = \sqrt{n + 1} | \varphi_{n+1,p} \rangle \\
a_G | \varphi_{n,p} \rangle = \sqrt{n} | \varphi_{n-1,p} \rangle \\
a_R^t | \varphi_{n,p} \rangle = \sqrt{p + 1} | \varphi_{n,p+1} \rangle \\
a_R | \varphi_{n,p} \rangle = \sqrt{p} | \varphi_{n,p-1} \rangle
\]

Independent oscillators can be solved as we know in their entirety.

The stationary states are given by a superposition of the modes.
Modes of an Infinite Chain of Coupled Oscillators: Phonons

\[ U(...) = \sum_{q=-\infty}^{+\infty} \frac{1}{2} m\omega_q^2 x_q^2 \]

\[ x_q(t) = x_q^M \cos(\omega t - \varphi_q) \]

Now imagine if neighboring particles exert attractive forces on each other:

\[ F_q = -m\omega_q^2 x_q - m\omega_1^2[ql + x_q - (q + 1)l - x_{q+1}] \]
\[ - m\omega_1^2[ql + x_q - (q - 1)l - x_{q-1}] \]
\[ = -m\omega_q^2 x_q - m\omega_1^2(x_q - x_{q+1}) - m\omega_1^2(x_q - x_{q-1}) \] (4)
Modes of an Infinite Chain of Coupled Oscillators: Phonons

The equation of motion becomes:

\[ m \frac{d^2}{dt^2} x_q(t) = -m\omega^2 x_q(t) - m\omega_1^2 \left[ 2x_q(t) - x_{q+1}(t) - x_{q-1}(t) \right] \]

\[ V(..., x_{-1}, x_0, x_1, ...) = \frac{1}{2} m\omega_1^2 \sum_{q=-\infty}^{+\infty} (x_q - x_{q+1})^2 \]

Imagine our chain as an infinitely long, macroscopic spring... We know that it can be compressed or expanded with waves travelling the length such that a single point along the spring experiences motion like:

\[ u(x, t) = \mu e^{i(kx-\Omega t)} + \mu^* e^{-i(kx-\Omega t)} \]

These solve the equation of motion if:

\[ -m\Omega^2 = -m\omega^2 - m\omega_1^2 \left[ 2 - e^{i\kappa l} - e^{-i\kappa l} \right] \]

In our problem we can use these simple solutions understanding that they can only be observed along discrete points:

\[ x_q(t) = u(ql, t) = \mu e^{i(kq l-\Omega t)} + \mu^* e^{-i(kq l-\Omega t)} \]

Which defines a dispersion relation:

\[ \Omega(k) = \sqrt{\omega^2 + 4\omega_1^2 \sin^2 \left( \frac{k l}{2} \right)} \]
Modes of an Infinite Chain of Coupled Oscillators: Phonons

\[ x_q(t) = u(ql, t) = \mu e^{i(kql - \Omega t)} + \mu^* e^{-i(kql - \Omega t)} \]

\[ \Omega(k) = \sqrt{\omega^2 + 4\omega_1^2 \sin^2 \left(\frac{k l}{2}\right)} \]

The out of phase component is determined by a sinusoidal wave with phase velocity:

\[ v_\phi(k) = \frac{\Omega(k)}{k} \]

What if wave vectors differ by an integral value related to the periodicity...

\[ k' = k + \frac{2n\pi}{l} \]

\[
\begin{align*}
\Omega(k') &= \Omega(k) \\
e^{i k' ql} &= e^{i k q l}
\end{align*}
\]

The motions of the oscillators are indistinguishable.

We only need consider values of \( k \) over the first Brillouin zone.

This “simple solution” describes all oscillators moving at the same frequency and amplitude, only out of phase. These are called “collective modes”.

\[ x_{[q_1 + q_2]}(t) = x_{q_1} \left( t - \frac{q_2 l}{v_\phi} \right) \]
Modes of an Infinite Chain of Coupled Oscillators: Phonons

\[ x_\phi(t) = u(ql, t) = \mu \, e^{i(kq - \Omega t)} + \mu^* \, e^{-i(kq - \Omega t)} \]

\[ \Omega(k) = \sqrt{\omega^2 + 4\omega_1^2 \sin^2 \left(\frac{kl}{2}\right)} \]

\[ v_\phi(k) = \frac{\Omega(k)}{k} \quad -\frac{\pi}{l} < k \leq \frac{\pi}{l} \]

We know that generally a wave packet carries a group velocity:

\[ v_G = \frac{d\Omega(k)}{dk} \]

The dispersion relation describes allowed frequencies. The mode with lowest frequency corresponds to an in-phase vibration of all oscillators. The highest describes a case where adjacent oscillators are entirely out-of-phase.
Modes of an Infinite Chain of Coupled Oscillators: Phonons

\[ m \frac{d^2}{dt^2} x_q(t) = -m\omega^2 x_q(t) - m\omega_1^2 \left[ 2x_q(t) - x_{q+1}(t) - x_{q-1}(t) \right] \]

Multiply both sides by: \( e^{-ik_q t} \)

While using:

\[
\sum_{q=-\infty}^{+\infty} x_{q+1} e^{-iql} = e^{ikl} \sum_{q=-\infty}^{+\infty} x_{q+1} e^{-i(q+1)kl} = \xi(k, t)
\]

\[
\sum_{q=-\infty}^{+\infty} x_q e^{-iql} = \xi(k, t)
\]

We obtain:

\[
\frac{\partial^2}{\partial t^2} \xi(k, t) = -\left[ \omega^2 + \omega_1^2(2 - e^{ikl} - e^{-ikl}) \right] \xi(k, t)
\]

The time evolution of \( \xi(k,t) \) is completely independent of \( \xi(k',t) \).

We were only able to generate \( \xi(k,t) \) because the chain was regular and infinite.
Modes of an Infinite Chain of Coupled Oscillators: Phonons

\[
\frac{\partial^2}{\partial t^2} \xi(k, t) = - \left[ \omega^2 + \omega_1^2 (2 - e^{ikl} - e^{-ikl}) \right] \xi(k, t)
\]

\[
\frac{\partial^2}{\partial t^2} \xi(k, t) = - \Omega^2(k) \xi(k, t)
\]

Let’s define an analogue for the momentum:

\[
\pi(k, t) = \sum_q p_q(t) e^{-iql}
\]

We can obtain the set of coupled equations of motion:

\[
\begin{cases}
    m \frac{\partial}{\partial t} \xi(k, t) = \pi(k, t) \\
    \frac{\partial}{\partial t} \pi(k, t) = - m\Omega^2(k) \xi(k, t)
\end{cases}
\]

If we differentiate both sides of the following term by term...

\[
\sum_{q = -\infty}^{+\infty} x_q(t) e^{-iqkl} = \xi(k, t)
\]

\(\xi\) and \(\pi\) are the normal variables in this case. We can describe the dynamical state of the system solely through them. Our discrete chain of coupled oscillators has been reduced a continuous system of independent oscillators where \(k\) acts as an index.
Modes of an Infinite Chain of Coupled Oscillators: Phonons

The Hamiltonian in terms of each particle is:

$$\sum_{q = -\infty}^{+\infty} x_q(t) e^{-iql} = \xi(k, t)$$

$$\pi(k, t) = \sum_{q} p_q(t) e^{-ikq}$$

Recognizing that the displacements and momenta are Fourier coefficients of the series defining $\xi$ and $\pi$, we can eventually reduce to:

$$\mathcal{H}(... x_{-1}, x_0, x_{+1}, ... p_{-1}, p_0, p_{+1}...) =$$

$$\sum_{q = -\infty}^{+\infty} \left[ \frac{1}{2m} p_q^2 + \frac{1}{2} m \omega^2 x_q^2 + \frac{1}{2} m \omega^2 (x_q - x_{q+1})^2 \right]$$

The Hamiltonian can be expressed as the integral of energies associated with fictitious uncoupled oscillators with continuous indices.
Quantum Treatment of the Infinite Chain of Oscillators

In the absence of coupling:

\[ H(\omega_1 = 0) = \sum_q \left[ \frac{1}{2} m\omega^2 X_q^2 + \frac{1}{2m} P_q^2 \right] \]

\[ = \sum_q H_q \]

We can use a different pair of creation/annihilation operators for each oscillator:

\[ a_q = \frac{1}{\sqrt{2}} \left[ \sqrt{\frac{m\omega}{\hbar}} X_q + \frac{i}{\sqrt{m\hbar\omega}} P_q \right] \]

\[ H_q = \frac{1}{2} (a_q a_q^\dagger + a_q^\dagger a_q) \hbar\omega = \left( a_q^\dagger a_q + \frac{1}{2} \right) \hbar\omega \]

\[ |\varphi_{n_q}\rangle = \frac{1}{\sqrt{(n_q)!}} (a_q^\dagger)^{n_q} |\varphi_0\rangle \]

The stationary states take on the following tensor product and energies:

\[ \cdots \otimes |\varphi_{n-1}\rangle \otimes |\varphi_0\rangle \otimes |\varphi_1\rangle \otimes \cdots \]

\[ E = \sum_q E^q_{n_q} = [\cdots + n_{-1} + n_0 + n_1 + \cdots] \hbar\omega \]

Aside from the ground state, energy levels of this system are infinitely degenerate.
Quantum Treatment of the Infinite Chain of Oscillators

Let’s add coupling:

\[ H(\omega_1 = 0) = \sum_q \left[ \frac{1}{2} m\omega^2 X_q^2 + \frac{1}{2m} P_q^2 \right] \]

\[ = \sum_q H_q \]

\[ H = H(\omega_1 = 0) + V \quad V = \frac{1}{2} m\omega_1^2 \sum_q (X_q - X_{q+1})^2 \]

The eigenstates of \( H \) are not eigenstates of \( V \):

\[ V = \frac{1}{4} \hbar \omega_1 \omega \sum_q \left( a_q + a_q^\dagger - a_{q+1} - a_{q+1}^\dagger \right)^2 \]

Any cross terms present in an expansion reveal that \( V \) can transfer excitation between different states.

Let’s simply introduce analogues of classical normal variables:

\[ \sum_{q = -\infty}^{+\infty} x_q(t) e^{-iqt} = \xi(k, t) \]

\[ \pi(k, t) = \sum_q p_q(t) e^{-ikl} \]

\[ \Xi(k) = \sum_q X_q e^{-ikl} \]

\[ \Pi(k) = \sum_q P_q e^{-ikl} \]
Quantum Treatment of the Infinite Chain of Oscillators

$$\Xi(k) = \sum_q X_q e^{-i qx}$$

Since $\xi$ and $\pi$ are complex their analogues are not Hermitian.

$$\Xi(-k) = \Xi^*(k)$$

$$\Pi(-k) = \Pi^*(k)$$

Let’s try to condense them for convenience:

$$a(k) = \frac{1}{\sqrt{2}} \left[ \beta(k) \Xi(k) + \frac{i}{\hbar \beta(k)} \Pi(k) \right]$$

$$\beta(k) = \sqrt{\frac{m \Omega(k)}{\hbar}}$$

$$a^*(k) = \frac{1}{\sqrt{2}} \left[ \beta(k) \Xi^*(k) - \frac{i}{\hbar \beta(k)} \Pi^*(k) \right]$$

$$[a(k), a(k')] = [a^*(k), a^*(k')] = 0$$

$$[a(k), a^* (k')] = \frac{2\pi}{l} \delta(k - k')$$
Quantum Treatment of the Infinite Chain of Oscillators

We previously saw:

$$\mathcal{H} = \frac{i}{2\pi} \int_{-\pi}^{+\pi} h(k) \, dk$$
$$h(k) = \frac{1}{2} m \Omega^2(k) |\xi(k, t)|^2 + \frac{1}{2m} |\pi(k, t)|^2$$

In the quantum treatment:

$$H(k) = \frac{1}{2m} \Pi(k) \Pi^\dagger(k) + \frac{1}{2} m \Omega^2(k) \Xi(k) \Xi^\dagger(k)$$

From what we’ve defined:

$$a(k) = \frac{1}{\sqrt{2}} \left[ \beta(k) \Xi(k) + \frac{i}{\hbar \beta(k)} \Pi(k) \right]$$
$$\beta(k) \Xi(k) = \frac{1}{\sqrt{2}} \left[ a(k) + a^\dagger(-k) \right]$$

$$a^\dagger(k) = \frac{1}{\sqrt{2}} \left[ \beta(k) \Xi^\dagger(k) - \frac{i}{\hbar \beta(k)} \Pi^\dagger(k) \right]$$
$$\frac{1}{\hbar \beta(k)} \Pi(k) = -\frac{i}{\sqrt{2}} \left[ a(k) - a^\dagger(-k) \right]$$
Quantum Treatment of the Infinite Chain of Oscillators

\[ H(k) = \frac{1}{2m} P(k) P^*(k) + \frac{1}{2} m\Omega^2(k) \Xi(k) \Xi^*(k) \]

\[ H(k) = \frac{1}{2} \hbar\Omega(k) \left[ a(k)a^*(k) + a^*(-k)a(-k) \right] \]

\[ H = \frac{l}{2\pi} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} dk \ H'(k) \quad H'(k) = \frac{1}{2} \hbar\Omega(k) \left[ a(k)a^*(k) + a^*(k)a(k) \right] \]

We can express the quantum Hamiltonian again in terms of creation and annihilation operators (different than the ones of a Harmonic oscillator), now defined over a continuous index.

\[ a(k) \left| 0 \right> = 0 \quad \text{Energy quanta are given by} \quad \Omega(k) = \sqrt{\omega^2 + 4\omega_1^2 \sin^2 \left(\frac{kl}{2} \right)} \]
Discussing Physical Phonons

Assume nuclei in a chain possess potential energy:

\[ U_N \approx \frac{1}{2} m \omega_1^2 \sum_q (x_q - x_{q+1})^2 \]

The dispersion is linear with \( k \) when \( k \) is small:

\[ |k| \ll \frac{1}{l} \quad \Omega(k) \approx \omega_1 |k| = v_s |k| \]

\[ v_s = \omega_1 l \]

The wavelength of motion must be much larger than atomic separation. The discrete nature of the chain can be neglected and the phase velocity is roughly constant. These are acoustic wavelengths and \( v_s \) is the speed of sound in a material.

We can use everything we just did, but must set \( \omega = 0 \) since nuclei are not truly bound to their equilibrium positions.

\[ \Omega(k) = \sqrt{\omega^2 + 4 \omega_1^2 \sin^2 \left( \frac{kl}{2} \right)} \]

\[ \Omega(k) = 2 \omega_1 \left| \sin \left( \frac{kl}{2} \right) \right| \]
Discussion & Questions