Lecture 16
Quantum field theory: from phonons to photons
In our survey of single- and “few”-particle quantum mechanics, it has been possible to work with individual constituent particles.

However, when the low energy excitations involve coherent collective motion of many individual particles – such as wave-like vibrations of an elastic solid...

...or where discrete underlying classical particles can not even be identified – such as the electromagnetic field,...

...such a representation is inconvenient or inaccessible.

In such cases, it is profitable to turn to a continuum formulation of quantum mechanics.

In the following, we will develop these ideas on background of the simplest continuum theory: lattice vibrations of atomic chain.

Provides platform to investigate the quantum electrodynamics – and paves the way to development of quantum field theory.
As a simplified model of (one-dimensional) crystal, consider chain of point particles, each of mass \( m \) (atoms), elastically connected by springs with spring constant \( k_s \) (chemical bonds).

Although our target will be to construct a *quantum* theory of vibrational excitations, it is helpful to first review classical system. Once again, to provide a bridge to the literature, we will follow the route of a Lagrangian formulation – but the connection to the Hamiltonian formulation is always near at hand!
For an $N$-atom chain, with periodic boundary conditions:

$$x_{N+1} = Na + x_1,$$

the Lagrangian is given by,

$$L = T - V = \sum_{n=1}^{N} \left[ \frac{m}{2} \ddot{x}_n^2 - \frac{k_s}{2} (x_{n+1} - x_n - a)^2 \right]$$

In real solids, inter-atomic potential is, of course, more complex – but at low energy (will see that) harmonic contribution dominates.

Taking equilibrium position, $\bar{x}_n \equiv na$, assume that $|x_n(t) - \bar{x}_n| \ll a$.

With $x_n(t) = \bar{x}_n + \phi_n(t)$, where $\phi_n$ is displacement from equilibrium,

$$L = \sum_{n=1}^{N} \left[ \frac{m}{2} \dot{\phi}_n^2 - \frac{k_s}{2} (\phi_{n+1} - \phi_n)^2 \right], \quad \phi_{N+1} = \phi_1$$
Classical chain: equations of motion

\[ L = \sum_{n=1}^{N} \left[ \frac{m}{2} \dot{\phi}_n^2 - \frac{k_s}{2} (\phi_{n+1} - \phi_n)^2 \right], \quad \phi_{N+1} = \phi_1 \]

- To obtain classical equations of motion from \( L \), we can make use of **Hamilton’s extremal principle**:
  
  For a point particle with coordinate \( x(t) \), the (Euler-Lagrange) equations of motion obtained from minimizing action

  \[ S[x] = \int dt \, L(\dot{x}, x) \quad \Rightarrow \quad \frac{d}{dt} (\partial_x L) - \partial_x L = 0 \]

  e.g. for a free particle in a harmonic oscillator potential \( V(x) = \frac{1}{2} kx^2 \),

  \[ L(\dot{x}, x) = \frac{1}{2} m\dot{x}^2 - \frac{1}{2} m\omega^2 x^2 \]

  and Euler-Lagrange equations translate to familiar equation of motion, \( m\ddot{x} = -kx \).
Classical chain: equations of motion

\[ L = \sum_{n=1}^{N} \left[ \frac{m}{2} \dot{\phi}_n^2 - \frac{k_s}{2} (\phi_{n+1} - \phi_n)^2 \right], \quad \phi_{N+1} = \phi_1 \]

- Minimization of the classical action for the chain, \( S = \int dt \, L[\dot{\phi}_n, \phi_n] \), leads to family of coupled Euler-Lagrange equations,

\[
\frac{d}{dt}(\partial_{\dot{\phi}_n} L) - \partial_{\phi_n} L = 0
\]

- With \( \partial_{\dot{\phi}_n} L = m \ddot{\phi}_n \) and \( \partial_{\phi_n} L = -k_s (\phi_n - \phi_{n+1}) - k_s (\phi_n - \phi_{n-1}) \), we obtain the discrete classical equations of motion,

\[
m \dddot{\phi}_n = -k_s (\phi_n - \phi_{n+1}) - k_s (\phi_n - \phi_{n-1}) \quad \text{for each } n
\]

- These equations describe the normal vibrational modes of the system. Setting \( \phi_n(t) = e^{i\omega t} \phi_n \), they can be written as

\[
(-m\omega^2 + 2k_s) \phi_n - k_s (\phi_{n+1} + \phi_{n-1}) = 0
\]
Classical chain: normal modes

\[
(-m\omega^2 + 2k_s)\phi_n - k_s(\phi_{n+1} + \phi_{n-1}) = 0
\]

- These equations have wave-like solutions (normal modes) of the form \(\phi_n = \frac{1}{\sqrt{N}}e^{ikna}\).

- With periodic boundary conditions, \(\phi_{n+N} = \phi_n\), we have \(e^{ikNa} = 1 = e^{2\pi mi}\). As a result, the wavenumber \(k = \frac{2\pi m}{Na}\) takes \(N\) discrete values set by integers \(N/2 \leq m < N/2\).

- Substituted into the equations of motion, we obtain

\[
(-m\omega^2 + 2k_s)\frac{1}{\sqrt{N}}e^{ikna} = k_s(e^{ika} + e^{-ika})\frac{1}{\sqrt{N}}e^{ikna}2k_s\cos(ka)
\]

- We therefore find that

\[
\omega = \omega_k = \sqrt{\frac{2k_s}{m}(1 - \cos(ka))} = 2\sqrt{\frac{k_s}{m}}|\sin(ka/2)|
\]
Classical chain: normal modes

\[ \omega_k = 2 \sqrt{\frac{k_s}{m}} |\sin(ka/2)| \]

- At low energies, \( k \to 0 \), (i.e. long wavelengths) the linear dispersion relation,

\[ \omega_k \approx v|k| \]

where \( v = a \sqrt{\frac{k_s}{m}} \) denotes the sound wave velocity, describes collective wave-like excitations of the harmonic chain.

- Before exploring quantization of these modes, let us consider how we can present the low-energy properties through a continuum theory.
Classical chain: continuum limit

\[ L = \sum_{n=1}^{N} \left[ \frac{m}{2} \dot{\phi}_n^2 - \frac{k_s}{2} \left( \phi_{n+1} - \phi_n \right)^2 \right] \]

- For low energy dynamics, relative displacement of neighbours is small, \( |\phi_{n+1} - \phi_n| \ll a \), and we can transfer to a continuum limit:

  \[ \phi_n \to \phi(x)|_{x=na}, \quad \phi_{n+1} - \phi_n \to a \partial_x \phi(x)|_{x=na}, \quad \sum_{n=1}^{N} \to \frac{1}{a} \int_{0}^{L=Na} dx \]

- Lagrangian \( L[\phi] = \int_{0}^{L} dx \mathcal{L}(\phi, \dot{\phi}) \), where **Lagrangian density**

\[ \mathcal{L}(\phi, \dot{\phi}) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} \left( \partial_x \phi \right)^2 \]
By turning to a continuum limit, we have succeeded in abandoning the \( N \)-point particle description in favour of one involving a set of continuous degrees of freedom, \( \phi(x) \) – known as a \textbf{(classical) field}.

Dynamics of \( \phi(x, t) \) specified by the Lagrangian and action functional

\[
L[\phi] = \int_0^{L=Na} dx \, L(\dot{\phi}, \phi), \quad S[\phi] = \int dt \, L[\phi]
\]

To obtain equations of motion, we have to turn again to the \textbf{principle of least action}.
Dynamics of harmonic chain

\[ \mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

- For a system with many degrees of freedom, we can still apply the same variational principle: \( \phi(x, t) \rightarrow \phi(x, t) + \epsilon \eta(x, t) \)

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} (S[\phi + \epsilon \eta] - S[\phi]) \equiv 0 = \int dt \int_0^L dx \left( \rho \ddot{\phi} \eta - \kappa_s a^2 \partial_x \phi \partial_x \eta \right)
\]

- Integrating by parts

\[
\int dt \int_0^L dx (\rho \dddot{\phi} - \kappa_s a^2 \partial_x^2 \phi) \eta = 0
\]

Since this relation must hold for any function \( \eta(x, t) \), we must have

\[ \rho \ddot{\phi} - \kappa_s a^2 \partial_x^2 \phi = 0 \]
Dynamics of harmonic chain

\[ \mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

- Classical equations of motion associated with Lagrangian density translate to **classical wave equation**:

\[ \rho \ddot{\phi} - \kappa_s a^2 \partial_x^2 \phi = 0 \]

- Solutions have the general form: \( \phi_+(x + vt) + \phi_-(x - vt) \) where \( v = a \sqrt{\kappa_s / \rho} = a \sqrt{k_s / m} \), and \( \phi_\pm \) are arbitrary smooth functions.

- Low energy elementary excitations are lattice vibrations, **sound waves**, propagating to left or right at constant velocity \( v \).

- Simple behaviour is consequence of simplistic definition of potential — no dissipation, etc.
Quantization of classical chain

- Is there a general methodology to quantize models of the form described by the atomic chain?

\[ \mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s \alpha^2}{2} (\partial_x \phi)^2 \]

- Recall the **canonical quantization procedure** for point particle mechanics:

1. Define canonical momentum: \( p = \partial_x \mathcal{L}(\dot{x}, x) \)
2. Construct Hamiltonian,

\[ \mathcal{H}(x, p) = p\dot{x} - \mathcal{L}(\dot{x}, x) \]

3. and, finally, promote conjugate coordinates \( x \) and \( p \) to operators with canonical commutation relations: \( [\hat{p}, \hat{x}] = -i\hbar \)
Is there a general methodology to quantize models of the form described by the atomic chain?

\[ \mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

**Canonical quantization procedure** for continuum theory follows same recipe:

1. Define canonical momentum: \( \pi = \partial_{\dot{\phi}} \mathcal{L}(\dot{\phi}, \phi) = \rho \dot{\phi} \)
2. Construct Hamiltonian, \( H[\phi, \pi] \equiv \int dx \mathcal{H}(\phi, \pi) \), where Hamiltonian density

\[ \mathcal{H}(\phi, \pi) = \pi \dot{\phi} - \mathcal{L}(\dot{\phi}, \phi) = \frac{1}{2\rho} \pi^2 + \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

3. Promote fields \( \phi(x) \) and \( \pi(x) \) to operators with canonical commutation relations: \( [\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar \delta(x - x') \)
Quantization of classical chain

\[ \hat{\mathcal{H}} = \int_0^L dx \left[ \frac{1}{2 \rho} \hat{\pi}^2 + \frac{k_s a^2}{2} (\partial_x \hat{\phi})^2 \right] \]

- For those uncomfortable with Lagrangian-based formulation, note that we could have obtained the Hamiltonian density by taking continuum limit of discrete Hamiltonian,

\[ \hat{\mathcal{H}} = \sum_{n=1}^N \left[ \frac{\hat{p}_n^2}{2m} + \frac{1}{2} k_s (\hat{\phi}_{n+1} - \hat{\phi}_n)^2 \right] \]

and the canonical commutation relations,

\[ [\hat{p}_m, \hat{\phi}_n] = -i\hbar \delta_{mn} \quad \Rightarrow \quad [\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar \delta(x - x') \]
Quantum chain

\[ \hat{H} = \int_0^L dx \left[ \frac{1}{2\rho} \hat{\pi}^2 + \frac{\kappa_s a^2}{2} (\partial_x \hat{\phi})^2 \right] \]

- Operator-valued functions, \( \hat{\phi} \) and \( \hat{\pi} \), referred to as quantum fields.
- Hamiltonian represents a formulation but not yet a solution.
- To address solution, helpful to switch to Fourier representation:

\[
\begin{align*}
\left\{ \begin{array}{c}
\hat{\phi}(x) \\
\hat{\pi}(x)
\end{array} \right\} &= \frac{1}{L^{1/2}} \sum_k e^{\{\pm ikx\}} \left\{ \begin{array}{c}
\hat{\phi}_k \\
\hat{\pi}_k
\end{array} \right\}, \\
\left\{ \begin{array}{c}
\hat{\phi}_k \\
\hat{\pi}_k
\end{array} \right\} &\equiv \frac{1}{L^{1/2}} \int_0^L dx \ e^{\{\mp ikx\}} \left\{ \begin{array}{c}
\hat{\phi}(x) \\
\hat{\pi}(x)
\end{array} \right\}
\end{align*}
\]

wavevectors \( k = 2\pi m/L, \ m \) integer.

- Since \( \phi(x) \) real, \( \hat{\phi}(x) \) is Hermitian, and \( \hat{\phi}_k = \hat{\phi}_{-k}^\dagger \) (similarly for \( \hat{\pi}_k \))

\[
\left[ \hat{\pi}_k, \hat{\phi}_k' \right] = -i\hbar \delta_{kk'} \ 	ext{(exercise)}
\]
Quantum chain

\[ \hat{H} = \int_0^L dx \left[ \frac{1}{2\rho} \hat{\pi}^2 + \frac{\kappa_s a^2}{2} (\partial_x \hat{\phi})^2 \right] \]

- In Fourier representation, \( \hat{\phi}(x) = \frac{1}{L^{1/2}} \sum_k e^{ikx} \hat{\phi}_k \),

\[
\int_0^L dx (\partial \hat{\phi})^2 = \sum_{k,k'} (ik\hat{\phi}_k)(ik'\hat{\phi}_{k'}) \frac{\delta_{k+k',0}}{L} \int_0^L dx e^{i(k+k')x} = \sum_k k^2 \hat{\phi}_k \hat{\phi}_{-k}
\]

- Together with parallel relation for \( \int_0^L dx \hat{\pi}^2 \),

\[ \hat{H} = \sum_k \left[ \frac{1}{2\rho} \hat{\pi}_k \hat{\pi}_{-k} + \frac{1}{2} \rho \omega_k^2 \hat{\phi}_k \hat{\phi}_{-k} \right] \]

\( \omega_k = \nu |k| \), and \( \nu = a(\kappa_s/\rho)^{1/2} \) is classical sound wave velocity.
Quantum chain

\[ \hat{H} = \sum_k \left[ \frac{1}{2\rho} \hat{\pi}_k \hat{\pi}_{-k} + \frac{1}{2} \rho \omega_k^2 \hat{\phi}_k \hat{\phi}_{-k} \right] \]

- Hamiltonian describes set of independent quantum harmonic oscillators (existence of indices \( k \) and \(-k\) is not crucial).
- Interpretation: classically, chain supports discrete set of wave-like excitations, each indexed by wavenumber \( k = 2\pi m/L \).
- In quantum picture, each of these excitations described by an oscillator Hamiltonian operator with a \( k \)-dependent frequency.
- Each oscillator mode involves all \( N \to \infty \) microscopic degrees of freedom – it is a \textbf{collective excitation} of the system.
The quantum harmonic oscillator describes motion of a single particle in a harmonic confining potential. Eigenvalues form a ladder of equally spaced levels, $\hbar \omega (n + 1/2)$.

Although we can find a coordinate representation of the states, $\langle x|n \rangle$, ladder operator formalism offers a second interpretation, and one that is useful to us now!

Quantum harmonic oscillator can be viewed as a simple system involving many featureless fictitious particles, each of energy $\hbar \omega$, created and annihilated by operators, $a^\dagger$ and $a$. 
Quantum harmonic oscillator: revisited

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 x^2 \]

- Specifically, introducing the operators,
  \[ a = \sqrt{\frac{m\omega}{2\hbar}} \left( x + i \frac{\hat{p}}{m\omega} \right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left( x - i \frac{\hat{p}}{m\omega} \right) \]
  which fulfil the commutation relations \([a, a^\dagger] = 1\), we have,

\[ \hat{H} = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right) \]

- The ground state (or vacuum) \(|0\rangle\) has energy \(E_0 = \hbar\omega / 2\) and is defined by the condition \(a|0\rangle = 0\).

- Excitations \(|n\rangle\) have energy \(E_n = \hbar\omega (n + 1/2)\) and are defined by action of the raising operator, \(|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle\), i.e. the “creation” of \(n\) fictitious particles.
Quantum chain

\[
\hat{H} = \sum_k \left[ \frac{1}{2\rho} \hat{\pi}_k \hat{\pi}_{-k} + \frac{1}{2} \rho \omega_k^2 \hat{\phi}_k \hat{\phi}_{-k} \right]
\]

- Inspired by ladder operator formalism for harmonic oscillator, set
  \[
  \hat{a}_k \equiv \sqrt{\frac{m \omega_k}{2\hbar}} \left( \hat{\phi}_k + \frac{i}{m \omega_k} \hat{\pi}_k \right), \quad \hat{a}_k^\dagger \equiv \sqrt{\frac{m \omega_k}{2\hbar}} \left( \hat{\phi}_{-k} - \frac{i}{m \omega_k} \hat{\pi}_k \right).
  \]

- Ladder operators obey the commutation relations:
  \[
  [a_k, a_{k'}^\dagger] = \frac{m \omega_k}{2\hbar} \frac{i}{m \omega_k} ([\hat{\pi}_{-k}, \hat{\phi}_{-k}] - [\hat{\phi}_k, \hat{\pi}_k]) \delta_{kk'}, \quad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = \]

- Hamiltonian assumes the diagonal form
  \[
  \hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right)
  \]
Quantum chain: phonons

\[ \hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) \]

- Low energy excitations of discrete atomic chain behave as discrete particles (even though they describe the collective motion of an infinite number of “fundamental” degrees of freedom) describing oscillator wave-like modes.

- These particle-like excitations, known as phonons, are characterised by wavevector \( k \) and have a linear dispersion, \( \omega_k = v|k| \).

- A generic state of the system is then given by

\[ |\{ n_k \} \rangle = \frac{1}{\sqrt{\prod_i n_i !}} (a_{k_1}^\dagger)^{n_1} (a_{k_2}^\dagger)^{n_2} \cdots |0 \rangle \]
Quantum chain: remarks

\[ \hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) \]

- In principle, we could now retrace our steps and express the elementary excitations, \( a_k^\dagger |0\rangle \), in terms of the continuum fields, \( \phi(x) \) (or even the discrete degrees of freedom \( \phi_n \)). **But why should we?**

- Phonon excitations represent perfectly legitimate (bosonic) particles which have physical manifestations which can be measured directly.

- We can regard phonons as “fundamental” and abandon microscopic degrees of freedom as being irrelevant on low energy scales!

- This hierarchy is generic, applying equally to high and low energy physics, e.g. electrons can be regarded as elementary collective excitation of a microscopic theory involving quarks, etc.
  
  for a discussion, see Anderson’s article “More is different”
Quantum chain: further remarks

$$\hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right), \quad \omega_k = v|k|$$

- **Universality**: At low energies, when phonon excitations involve long wavelengths ($k \to 0$), modes become insensitive to details at atomic scale justifying our crude modelling scheme.

- As $k \to 0$, phonon excitations incur vanishingly small energy – the spectrum is said to be “massless”.

- Such behaviour is in fact generic: the breaking of a continuous symmetry (in this case, translation) always leads to massless collective excitations – known as **Goldstone modes**.
Quantization of the harmonic chain: recap

Starting with the classical Lagrangian for a harmonic chain,

\[ L = \sum_{n=1}^{N} \left[ \frac{m}{2} \phi_n^2 - \frac{k_s}{2} (\phi_{n+1} - \phi_n)^2 \right], \quad \phi_{N+1} = \phi_1 \]

we showed that the normal mode spectrum was characterised by a linear low energy dispersion, \( \omega_k = v|k| \), where \( v = a \sqrt{k_s/m} \) denotes the classical sound wave velocity.

To prepare for our study of the quantization of the EM field, we then turned from the discrete to the continuum formulation of the classical Lagrangian setting \( L[\phi] = \int_0^L dx \mathcal{L}(\dot{\phi}, \phi) \), where

\[ \mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

\( \rho = m/a \) is mass per unit length and \( \kappa_s = k_s/a \).
Quantization of harmonic chain: recap

\[
\mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2
\]

- From the minimisation of the classical action, \( S[\phi] = \int dt \, L[\phi] \), the Euler-Lagrange equations recovered the classical wave equation,

\[
\rho \ddot{\phi} = \kappa_s a^2 \partial_x^2 \phi
\]

with the solutions: \( \phi_+(x + vt) + \phi_-(x - vt) \)

- As expected from the discrete formulation, the low energy excitations of the chain are lattice vibrations, sound waves, propagating to left or right at constant velocity \( v \).
Quantization of harmonic chain: recap

To quantize the classical theory, we developed the canonical quantization procedure:

\[ \mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

1. Define canonical momentum: \( \pi = \partial_{\dot{\phi}} \mathcal{L}(\dot{\phi}, \phi) = \rho \dot{\phi} \)

2. Construct Hamiltonian, \( H[\phi, \pi] \equiv \int dx \, \mathcal{H}(\phi, \pi) \), where Hamiltonian density

\[ \mathcal{H}(\phi, \pi) = \pi \dot{\phi} - \mathcal{L}(\dot{\phi}, \phi) = \frac{1}{2\rho} \pi^2 + \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \]

3. Promote fields \( \phi(x) \) and \( \pi(x) \) to operators with canonical commutation relations: \( [\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar \delta(x - x') \)
Quantization of harmonic chain: recap

![Quantization of harmonic chain: recap](image)

\[\hat{H} = \int_0^L dx \left[ \frac{1}{2\rho} \hat{\pi}^2 + \frac{\kappa_s a^2}{2} (\partial_x \hat{\phi})^2 \right]\]

- To find the eigenmodes of the quantum chain, we then turned to the Fourier representation:

\[
\begin{align*}
\hat{\phi}(x) &= \frac{1}{L^{1/2}} \sum_k \cos \{\pm ikx\} \hat{\phi}_k \\
\hat{\pi}(x) &= \frac{1}{L^{1/2}} \sum_k \sin \{\pm ikx\} \hat{\pi}_k
\end{align*}
\]

with \( k = \frac{2\pi m}{L}, \) \( m \) integer, whereupon the Hamiltonian takes the “near-diagonal” form,

\[\hat{H} = \sum_k \left[ \frac{1}{2\rho} \hat{\pi}_k \hat{\pi}_{-k} + \frac{1}{2} \frac{\omega_k^2}{\rho} \hat{\phi}_k \hat{\phi}_{-k} \right]\]
Quantization of harmonic chain: recap

\[ \hat{H} = \sum_k \left[ \frac{1}{2\rho} \hat{\pi}_k \hat{\pi}_{-k} + \frac{1}{2} \rho \omega_k^2 \hat{\phi}_k \hat{\phi}_{-k} \right] \]

- \( \hat{H} \) describes set of independent oscillators with \( k \)-dependent frequency. Each mode involves all \( N \to \infty \) microscopic degrees of freedom – it is a collective excitation.

- Inspired by ladder operator formalism, setting

\[
\hat{a}_k \equiv \sqrt{\frac{m\omega_k}{2\hbar}} \left( \hat{\phi}_k + \frac{i}{m\omega_k} \hat{\pi}_{-k} \right), \quad \hat{a}_k^\dagger \equiv \sqrt{\frac{m\omega_k}{2\hbar}} \left( \hat{\phi}_{-k} - \frac{i}{m\omega_k} \hat{\pi}_k \right).
\]

where \( [a_k, a_{k'}^\dagger] = \delta_{kk'} \), Hamiltonian takes diagonal form,

\[ \hat{H} = \sum_k \hbar \omega_k \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) \]
Quantization of harmonic chain: recap

\[ \hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) \]

- Low energy excitations of discrete atomic chain behave as discrete particles (even though they describe collective motion of an infinite number of “fundamental” degrees of freedom).

- These particle-like excitations, known as phonons, are characterised by wavevector \( k \) and have a linear dispersion, \( \omega_k = v|k| \).

- A generic state of the system is then given by

\[
|\{n_k\}\rangle = \frac{1}{\sqrt{\prod_i n_i!}} (a_{k_1}^\dagger)^{n_1} (a_{k_2}^\dagger)^{n_2} \cdots |0\rangle
\]
In theory, we could now retrace our steps and express the elementary excitations, \( a_k^\dagger |0\rangle \), in terms of continuum fields, \( \phi(x) \) (or even the discrete degrees of freedom \( \phi_n \)). **But why should we?**

Phonon excitations represent perfectly “legitimate” particles which have physical manifestations which can be measured directly – we can regard phonons are “fundamental” and abandon microscopic degrees of freedom as being irrelevant on low energy scales!

If fact, such a heirarchy is quite generic in physics: “Fundamental” particles are always found to be collective excitations of some yet more “fundamental” theory!

see Anderson’s article “More is different” (now on website!)
Quantization of harmonic chain: second quantization

But when we studied identical quantum particles we declared that all fundamental particles can be classified as bosons or fermions – so what about the quantum statistics of phonons?

- In fact, commutation relations tell us that phonons are **bosons**: Using the relation \([a_{k}^\dagger, a_{k'}^\dagger] = 0\), we can see that the many-body wavefunction is symmetric under particle exchange,

  \[
  |k_1, k_2\rangle = a_{k_1}^\dagger a_{k_2}^\dagger |0\rangle = a_{k_2}^\dagger a_{k_1}^\dagger |0\rangle = |k_2, k_1\rangle
  \]

- In fact, the commutation relations of the operators circumvent need to explicitly symmetrize the many-body wavefunction,

  \[
  |k_1, k_2\rangle = a_{k_1}^\dagger a_{k_2}^\dagger |0\rangle = \frac{1}{2} \left( a_{k_1}^\dagger a_{k_2}^\dagger + a_{k_2}^\dagger a_{k_1}^\dagger \right) |0\rangle
  \]

  is already symmetrized!

- Again, this property is generic and known as **second quantization**.
Quantization of harmonic chain: further lessons

\[ \hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right), \quad \omega_k = v |k| \]

- **Universality**: At low energies, when phonon excitations involve long wavelengths \((k \to 0)\), modes become insensitive to details at atomic scale justifying crude modelling scheme.

- As \(k \to 0\), phonon excitations incur vanishingly small energy – the spectrum is said to be “massless”.

- Again, such behaviour is generic: the breaking of a continuous symmetry (in this case, translation) always leads to massless collective excitations – known as **Goldstone modes**.
Our analysis focussed on longitudinal vibrations of one-dimensional chain. In three-dimensions, each mode associated with three possible polarizations, \( \lambda \): two transverse and one longitudinal.

Taking into account all polarizations

\[
\hat{H} = \sum_{\mathbf{k}, \lambda} \hbar \omega_{\mathbf{k}\lambda} \left( a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}, \lambda} + \frac{1}{2} \right)
\]

where \( \omega_{\mathbf{k}\lambda} = v_{\lambda} |\mathbf{k}| \) and \( v_{\lambda} \) are respective sound wave velocities.

Let us apply this result to obtain internal energy and specific heat due to phonons.
Example: Debye theory of solids

- For equilibrium distribution, average phonon occupancy of state \((k, \lambda)\) given by Bose-Einstein distribution, \(n_B(\hbar \omega_k) \equiv \frac{1}{e^{\hbar \omega_k / k_B T} - 1} \).

- The internal energy therefore given by

\[
E = \sum_{k\lambda} \hbar \omega_k \left[ \frac{1}{e^{\hbar \omega_k / k_B T} - 1} + \frac{1}{2} \right]
\]

- In thermodynamic limit, \(\sum_k \rightarrow \frac{L^3}{(2\pi)^3} \int_0^{k_D} d^3k = \frac{L^3}{2\pi^2} \int_0^{k_D} k^2 dk\), with cut-off \(k_D\) fixed by ensuring that total number of modes matches degrees of freedom, \(\frac{1}{(2\pi/L)^3} \frac{4}{3} \pi k_D^3 = N \equiv \frac{L^3}{a^3}\), i.e. \(k_D^3 = \frac{6\pi^2}{a^3}\).

- Dropping zero point fluctuations, if \(v_\lambda = v\) (independent of \(\lambda\)), internal energy/particle given by

\[
\varepsilon \equiv \frac{E}{N} = 3 \times \frac{a^3}{2\pi^2} \frac{9}{k_D^3} \int_0^{k_D} k^2 dk \frac{\hbar v k}{e^{\hbar v k / k_B T} - 1}
\]
Example: Debye theory of solids

\[ \varepsilon \equiv \frac{E}{N} = \frac{9}{k_D^3} \int_0^{k_D} k^2 \, dk \frac{\hbar v k}{e^{\hbar v k / k_B T} - 1}. \]

- Defining Debye temperature, \( k_B T_D = \hbar v k_D \),

\[ \varepsilon = 9k_B T \left( \frac{T}{T_D} \right)^3 \int_0^{T_D / T} \frac{z^3 \, dz}{e^z - 1} \]

- Leads to specific heat per particle,

\[ c_V = \partial_T \varepsilon = 9k_B \left( \frac{T}{T_D} \right)^3 \int_0^{T_D / T} \frac{z^4 \, dz}{(e^z - 1)^2} = \begin{cases} 3k_B & T \gg T_D \\ A T^3 & T \ll T_D \end{cases} \]
Example: Debye theory of solids

\[ c_V = \partial_T \varepsilon = 9k_B \left( \frac{T}{T_D} \right)^3 \int_0^{T_D/T} \frac{z^4 \, dz}{(e^z - 1)^2} = 3k_B \frac{T}{T_D} \quad \text{for } T \gg T_D \]

\[ A T^3 \quad \text{for } T \ll T_D \]

Fit of silver specific heat data to the Debye curve with \( T_D = 215 \text{ K} \).
Lecture 17

Quantization of the Electromagnetic Field
As with harmonic chain, electromagnetic (EM) field satisfies wave equation in vacua.

\[ \frac{1}{c^2} \dddot{E} = \nabla^2 E, \quad \frac{1}{c^2} \dddot{B} = \nabla^2 B \]

Generality of quantization procedure for chain suggests that quantization of EM field should proceed in analogous manner.

However, gauge freedom of vector potential introduces redundant degrees of freedom whose removal on quantum level is not completely straightforward.

Therefore, to keep discussion simple, we will focus on a simple one-dimensional waveguide geometry to illustrate main principles.
In vacuum, Lagrangian density of EM field given by

\[ \mathcal{L} = -\frac{1}{4\mu_0} F_{\mu\nu} F^{\mu\nu} \]

where \( F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \) denotes EM field tensor, \( \mathbf{E} = \dot{\mathbf{A}} \) is electric field, and \( \mathbf{B} = \nabla \times \mathbf{A} \) is magnetic field.

In absence of current/charge sources, it is convenient to adopt Coulomb gauge, \( \nabla \cdot \mathbf{A} = 0 \), with the scalar component \( \phi = 0 \), when

\[ L[\dot{A}, A] = \int d^3x \mathcal{L} = \frac{1}{2\mu_0} \int d^3x \left[ \frac{1}{c^2} \dot{A}^2 - (\nabla \times A)^2 \right] \]

Corresponding classical equations of motion lead to wave equation

\[ \frac{1}{c^2} \ddot{A} = \nabla^2 A \quad \leftrightarrow \quad \partial_\mu F^{\mu\nu} = 0 \]
Classical theory of electromagnetic field

$$L[\dot{\mathbf{A}}, \mathbf{A}] = \frac{1}{2\mu_0} \int d^3x \left[ \frac{1}{c^2} \dot{\mathbf{A}}^2 - (\nabla \times \mathbf{A})^2 \right]$$

- Structure of Lagrangian mirrors that of harmonic chain:

$$L[\dot{\phi}, \phi] = \int dx \left[ \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s a^2}{2} (\partial_x \phi)^2 \right]$$

- By analogy with chain, to quantize classical field, we should elevate fields to operators and switch to Fourier representation.

- However, in contrast to chain, we are now dealing with
  (i) a full three-dimensional Laplacian acting upon...
  (ii) the vector field $\mathbf{A}$ that is...
  (iii) subject to the constraint $\nabla \cdot \mathbf{A} = 0$. 
Classical theory of EM field: waveguide

\[ L[\dot{\mathbf{A}}, \mathbf{A}] = \frac{1}{2\mu_0} \int d^3x \left[ \frac{1}{c^2} \dot{\mathbf{A}}^2 - (\nabla \times \mathbf{A})^2 \right] \]

- We can circumvent difficulties by considering simplified geometry which reduces complexity of eigenvalue problem.

- In a strongly anisotropic waveguide, the low frequency modes become quasi one-dimensional, specified by a single wavevector, \( k \).

- For a classical EM field, the modes of the cavity must satisfy boundary conditions commensurate with perfectly conducting walls, \( \hat{e}_n \times \mathbf{E} \equiv \mathbf{E}_\parallel \big|_{\text{boundary}} = 0 \) and \( \hat{e}_n \cdot \mathbf{B} \equiv \mathbf{B}_\perp \big|_{\text{boundary}} = 0 \).
For waveguide, general vector potential configuration may be expanded in eigenmodes of classical wave equation,

\[- \nabla^2 u_k(x) = \lambda_k u_k(x)\]

where \(u_k\) are real and orthonormal, \(\int d^3x u_k \cdot u_{k'} = \delta_{kk'}\) (cf. Fourier mode expansion of \(\hat{\phi}(x)\) and \(\hat{\pi}(x)\)).

With boundary conditions \(u_\parallel|_{\text{boundary}} = 0\) (cf. \(E_\parallel|_{\text{boundary}} = 0\)), for anisotropic waveguide with \(L_z < L_y \ll L_x\), smallest \(\lambda_k\) are those with \(k_z = 0\), \(k_y = \pi/L_y\), and \(k_x \equiv k \ll L_{z,y}^{-1}\),

\[u_k = \frac{2}{\sqrt{V}} \sin(\pi y/L_y) \sin(kx) \hat{e}_z, \quad \lambda_k = k^2 + \left(\frac{\pi}{L_y}\right)^2\]
Classical theory of EM field: waveguide

\[ L[\dot{\mathbf{A}}, \mathbf{A}] = \frac{1}{2\mu_0} \int d^3x \left[ \frac{1}{c^2} \dot{\mathbf{A}}^2 - (\nabla \times \mathbf{A})^2 \right] \]

- Setting \( \mathbf{A}(x, t) = \sum_k \alpha_k(t) \mathbf{u}_k(x) \), with \( k = \pi n/L \) and \( n \) integer, and using orthonormality of functions \( \mathbf{u}_k(x) \),

\[ L[\dot{\alpha}, \alpha] = \frac{1}{2\mu_0} \sum_k \left[ \frac{1}{c^2} \dot{\alpha}_k^2 - \lambda_k \alpha_k^2 \right] \]

- i.e. system described in terms of independent dynamical degrees of freedom, with coordinates \( \alpha_k \) (cf. atomic chain),

\[ L[\dot{\phi}, \phi] = \int dx \left[ \frac{\rho}{2} \dot{\phi}^2 - \frac{\kappa_s}{2} \partial_x^2 \phi^2 \right] \]
Quantization of classical EM field

\[ L[\dot{\alpha}, \alpha] = \frac{1}{2\mu_0} \sum_k \left[ \frac{1}{c^2} \dot{\alpha}_k^2 - \lambda_k \alpha_k^2 \right] \]

1. Define canonical momenta \( \pi_k = \partial_{\dot{\alpha}_k} L = \epsilon_0 \dot{\alpha}_k \), where \( \epsilon_0 = \frac{1}{\mu_0 c^2} \) is vacuum permittivity

\[
H = \sum_k \pi_k \dot{\alpha}_k - L = \sum_k \left( \frac{1}{2\epsilon_0} \pi_k^2 + \frac{1}{2} \epsilon_0 c^2 \lambda_k \alpha_k^2 \right)
\]

2. Quantize operators: \( \alpha_k \to \hat{\alpha}_k \) and \( \pi_k \to \hat{\pi}_k \).

3. Declare commutation relations: \( [\hat{\pi}_k, \hat{\alpha}_{k'}] = -i\hbar \delta_{kk'} \):

\[
\hat{H} = \sum_k \left[ \frac{\hat{\pi}_k^2}{2\epsilon_0} + \frac{1}{2} \epsilon_0 \omega_k^2 \hat{\alpha}_k^2 \right], \quad \omega_k^2 = c^2 \lambda_k
\]
Quantization of classical EM field

\[
\hat{H} = \sum_k \left[ \frac{\hat{\pi}_k^2}{2\epsilon_0} + \frac{1}{2}\epsilon_0\omega_k^2 \hat{\alpha}_k^2 \right], \quad \omega_k^2 = c^2 \lambda_k
\]

- Following analysis of atomic chain, if we introduce ladder operators,

\[
a_k = \sqrt{\frac{\epsilon_0\omega_k}{2\hbar}} \left( \hat{\alpha}_k + \frac{i}{\epsilon_0\omega_k} \hat{\pi}_k \right), \quad a_k^\dagger = \sqrt{\frac{\epsilon_0\omega_k}{2\hbar}} \left( \hat{\alpha}_k - \frac{i}{\epsilon_0\omega_k} \hat{\pi}_k \right)
\]

with \([a_k, a_{k'}^\dagger] = \delta_{kk'}\), Hamiltonian takes familiar form,

\[
\hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right)
\]

- For waveguide of width \(L_y\), \(\hbar \omega_k = c[k^2 + (\pi/L_y)^2]^{1/2}\).
Quantization of EM field: remarks

\[ \hat{H} = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) , \quad |n_k\rangle = \frac{1}{\sqrt{n_k!}} (a_k^\dagger)^{n_k} |\Omega\rangle \]

- Elementary particle-like excitations of EM field, known as photons, are created or annihilated by operators \( a_k^\dagger \) and \( a_k \).

\[ a_k^\dagger |n_k\rangle = \sqrt{n_k + 1} |n_k + 1\rangle , \quad a_k |n_k\rangle = \sqrt{n_k} |n_k - 1\rangle \]

- Unfamiliar dispersion relation

\[ \omega_k = c [k^2 + (\pi / L_y)^2]^{1/2} \]

is manifestation of waveguide geometry – for \( k \gg L_y^{-1} \), recover expected linear dispersion,

\[ \omega_k \simeq c |k| \]
So far, we have considered EM field quantization for a waveguide – what happens in a three-dimensional cavity or free space?

- For waveguide geometry, we have seen that $\hat{A}(x) = \sum_{k} \hat{\alpha}_{k} u_{k}$ where

$$\hat{\alpha}_{k} = \sqrt{\frac{\hbar}{2\varepsilon_{0}\omega_{k}}} (a_{k} + a_{k}^{\dagger})$$

- In a three-dimensional cavity, vector potential can be expanded in plane wave modes as

$$\hat{A}(x) = \sum_{k\lambda=1,2} \sqrt{\frac{\hbar}{2\varepsilon_{0}\omega_{k}V}} \left[ \hat{e}_{k\lambda} a_{k\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{e}_{k\lambda}^{*} a_{k\lambda}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}} \right]$$

where $V$ is volume, $\omega_{k} = c|\mathbf{k}|$, and $\hat{e}_{k\lambda}$ denote two sets of (generally complex) normalized polarization vectors ($\hat{e}_{k\lambda}^{*} \cdot \hat{e}_{k\lambda} = 1$).
Quantization of EM field: generalization

\[ \hat{A}(x) = \sum_{k\lambda=1,2} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_k V}} \left[ \hat{e}_{k\lambda} a_{k\lambda} e^{ik\cdot x} + \hat{e}_{k\lambda}^* a_{k\lambda}^\dagger e^{-ik\cdot x} \right] \]

- Coulomb gauge condition, \( \nabla \cdot A = 0 \), requires \( \hat{e}_{k\lambda} \cdot k = \hat{e}_{k\lambda}^* \cdot k = 0 \).

- If vectors \( \hat{e}_{k\lambda} \) real (in-phase), polarization linear, otherwise circular – typically define \( \hat{e}_{k\lambda} \cdot \hat{e}_{k\mu} = \delta_{\mu\nu} \).

- Finally, operators obey (bosonic) commutation relations,

\[ [a_{k\lambda}, a_{k'\lambda'}^\dagger] = \delta_{k,k'} \delta_{\lambda\lambda'} \]

while \( [a_{k\lambda}, a_{k'\lambda'}] = 0 = [a_{k\lambda}^\dagger, a_{k'\lambda'}^\dagger] \).
Quantization of EM field: generalization

\[ \hat{A}(x) = \sum_{\kappa\lambda=1,2} \sqrt{\frac{\hbar}{2\epsilon_0\omega_k V}} \left[ \hat{e}_{k\lambda} a_{k\lambda} e^{ik \cdot x} + \hat{e}^*_{k\lambda} a^\dagger_{k\lambda} e^{-ik \cdot x} \right] \]

- With these definitions, the photon Hamiltonian then takes the form

\[ \hat{H} = \sum_{\kappa\lambda} \hbar \omega_k \left[ a^\dagger_{k\lambda} a_{k\lambda} + 1/2 \right] \]

- Defining vacuum, \(|\Omega\rangle\), eigenstates involve photon number states,

\[ |\{n_{k\lambda}\} \rangle = \frac{1}{\sqrt{\prod_{\kappa\lambda} n_{k\lambda}!}} (a^\dagger_{k1\lambda})^{n_{k1\lambda}} (a^\dagger_{k2\lambda})^{n_{k2\lambda}} \cdots |\Omega\rangle \]

N.B. commutation relations of bosonic operators ensures that many-photon wavefunction symmetrical under exchange.
Momentum carried by photon field

- Classical EM field carries linear momentum density, $S/c^2$ where $S = \mathbf{E} \times \mathbf{B}/\mu_0$ denotes Poynting vector, i.e. total momentum

$$
\mathbf{P} = \int d^3x \frac{1}{c^2} S = -\epsilon_0 \int d^3x \dot{\mathbf{A}}(\mathbf{x}, t) \times (\nabla \times \mathbf{A}(\mathbf{x}, t))
$$

- After quantization, find (exercise)

$$
\hat{\mathbf{P}} = \sum_{\mathbf{k}, \lambda} \hbar \mathbf{k} a_{\mathbf{k}, \lambda}^{\dagger} a_{\mathbf{k}, \lambda} \\
\text{i.e. } \hat{\mathbf{P}}|\mathbf{k}, \lambda\rangle = \hat{\mathbf{P}} a_{\mathbf{k}, \lambda}^{\dagger} |\Omega\rangle = \hbar \mathbf{k}|\mathbf{k}, \lambda\rangle \text{ (for both } \lambda = 1, 2).$$
Angular momentum carried by photon field

- Angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{P}$ includes intrinsic component,

$$M = - \int d^3 \mathbf{x} \mathbf{A} \times \mathbf{A} \leftrightarrow \hat{M} = -i\hbar \sum_k \hat{e}_k \left[ a_{k1}^{\dagger} a_{k2} - a_{k2}^{\dagger} a_{k1} \right]$$

- Defining creation operators for right/left circular polarization,

$$a_{kR}^{\dagger} = \frac{1}{\sqrt{2}} (a_{k1}^{\dagger} + ia_{k2}^{\dagger}), \quad a_{kL}^{\dagger} = \frac{1}{\sqrt{2}} (a_{k1}^{\dagger} - ia_{k2}^{\dagger})$$

find that

$$\hat{M} = \sum_k \hbar \hat{e}_k \left[ a_{kR}^{\dagger} a_{kR} - a_{kL}^{\dagger} a_{kL} \right]$$

- Therefore, since $\hat{e}_k \cdot \hat{M} | \mathbf{k}, \text{R/L} \rangle = \pm \hbar | \mathbf{k}, \text{R/L} \rangle$, we conclude that photons carry intrinsic angular momentum $\pm \hbar$ (known as helicity), oriented parallel/antiparallel to direction of momentum propagation.
Casimir effect

\[ \hat{H} = \sum_{k\lambda} \hbar \omega_k \left[ a_{k\lambda}^{\dagger} a_{k\lambda} + 1/2 \right] \]

- As with harmonic chain, quantization of EM field \( \leadsto \) zero-point fluctuations with physical manifestations.

- Consider two metallic plates, area \( A \), separated by distance \( d \) – quantization of EM field leads to vacuum energy/unit area

\[
\frac{\langle E \rangle}{A} = 2 \times \int \frac{d^2 k_{\perp}}{(2\pi)^2} \sum_{n=1}^{\infty} \frac{\hbar \omega_{k_{\perp} n}}{2} = -\frac{\pi^2}{720} \frac{\hbar c}{d^3}, \quad \omega_{k_{\perp} n} = c \sqrt{k_{\perp}^2 + \left(\frac{\pi n}{d}\right)^2}
\]

- Field quantization results in attractive (Casimir) force/unit area,

\[
\frac{F_C}{A} = - \frac{\partial_d \langle E \rangle}{A} = -\frac{\pi^2}{240} \frac{\hbar c}{d^4}
\]
Starting with continuum field theory of the classical harmonic chain, we have developed a general quantization programme. From this programme, we find that the low-energy elementary excitations of the chain are described by (bosonic) particle-like collective excitations known as **phonons**.

In three-dimensional system, modes acquire polarization index, \( \lambda \).
Quantum field theory: summary

- Starting with continuum field theory of EM field for waveguide,

\[ L[\dot{\alpha}, \alpha] = \sum_k \left[ \frac{1}{c^2} \dot{\alpha}^2 - \lambda_k \alpha_k^2 \right] \]

we applied quantization procedure to establish quantum theory.

- These studies show that low-energy excitations of EM field described by (bosonic) particle-like modes known as \textit{photons},

\[ \hat{H} = \sum_k \hbar \omega_k (a_k^{\dagger} a_k + 1/2), \quad \omega_k = c(k^2 + (\pi/L_y)^2)^{1/2} \]

- In three-dimensional system modes acquire polarization index, \( \lambda \).

\[ \hat{H} = \sum_{k\lambda} \hbar \omega_k (a_{k\lambda}^{\dagger} a_{k\lambda} + 1/2), \quad \omega_k = c|k| \]
As a final example of field quantization, which revises operator methods and spin angular momentum, we close this section by considering the quantum mechanical spin chain.
In correlated electron systems Coulomb interaction can result in electrons becoming localized – the **Mott transition**.

However, in these insulating materials, the spin degrees of freedom carried by the constituent electrons can remain mobile – such systems are described by quantum magnetic models, where **exchange couplings** $J_{mn}$ denote matrix elements coupling local moments at lattice sites $m$ and $n$. 

$$\hat{H} = \sum_{m\neq n} J_{mn} \hat{S}_m \cdot \hat{S}_n$$
Spin wave theory

\[ \hat{H} = \sum_{m \neq n} J_{mn} \hat{S}_m \cdot \hat{S}_n \]

- Since matrix elements \( J_{mn} \) decay rapidly with distance, we may restrict attention to just neighbouring sites, \( J_{mn} = J_\delta_{m,n \pm 1} \).

- Although \( J \) typically positive (leading to antiferromagnetic coupling), here we consider them negative leading to ferromagnetism – i.e. neighbouring spins want to lie parallel.

- Consider then the 1d spin \( S \) quantum Heisenberg ferromagnet,

\[ \hat{H} = -J \sum_m \hat{S}_m \cdot \hat{S}_{m+1} \]

where \( J > 0 \), and spins obey spin algebra, \([\hat{S}_m^\alpha, \hat{S}_n^\beta] = i\hbar \delta_{mn} \epsilon^{\alpha\beta\gamma} \hat{S}_m^\gamma\).
Spin wave theory

\[ \hat{H} = -J \sum_m \hat{S}_m \cdot \hat{S}_{m+1} \]

- As a strongly interacting quantum system, for a general spin \( S \), the quantum magnetic Hamiltonian is not easily addressed. However, for large spin \( S \), we can develop a “semi-classical” expansion:

- In problem set I, we developed a representation of the quantum spin algebra, \([\hat{S}_m^+, \hat{S}_n^-] = 2\hbar \hat{S}^z \delta_{mn}\), using raising and lowering (ladder) operators – the Holstein-Primakoff spin representation,

\[
\begin{align*}
\hat{S}^z_m &= \hbar (S - a_m^\dagger a_m) \\
\hat{S}^-_m &= \hbar \sqrt{2S} a_m^\dagger \left(1 - \frac{a_m^\dagger a_m}{2S}\right)^{1/2} \approx \hbar \sqrt{2S} a_m^\dagger + O(S^{-1/2}) \\
\hat{S}^+_m &= (\hat{S}^-_m)^\dagger \approx \hbar \sqrt{2S} a_m + O(S^{-1/2})
\end{align*}
\]

where, as usual, \([a_m, a_n^\dagger] = \delta_{mn}\).
Spin wave theory

\[ \hat{H} = -J \sum_m \hat{S}_m \cdot \hat{S}_{m+1} \]

• Defining spin raising and lowering operators, \( \hat{S}_m^\pm = \hat{S}_m^x \pm i\hat{S}_m^y \),

\[
\hat{H} = -J \sum_m \left\{ \frac{1}{2} (\hat{S}_m^+ \hat{S}_{m+1}^- + \hat{S}_m^- \hat{S}_{m+1}^+) + \hat{S}_m^z \hat{S}_{m+1}^z \right\} + \frac{1}{2} (\hat{S}_m^+ \hat{S}_{m+1}^- + \hat{S}_m^- \hat{S}_{m+1}^+) 
\]

• Using Holstein-Primakoff transformation,

\[
\hat{S}_m^z = \hbar (S - a_m^\dagger a_m), \quad \hat{S}_m^- \simeq \hbar \sqrt{2S} a_m^\dagger, \quad \hat{S}_m^+ \simeq \hbar \sqrt{2S} a_m 
\]

expansion to quadratic order in raising and lowering operators gives,

\[
\hat{H} \simeq -JN\hbar^2 S^2 - J\hbar^2 S \sum_m (a_m a_{m+1}^\dagger + a_m^\dagger a_{m+1} - a_m^\dagger a_m - a_{m+1}^\dagger a_{m+1}) 
\]

\[
\hat{H} = -JN\hbar^2 S^2 + J\hbar^2 S \sum_m (a_{m+1}^\dagger - a_m^\dagger)(a_{m+1} - a_m) + O(S^0) 
\]
Spin wave theory

\[ \hat{H} = -JN\hbar^2 S^2 + \frac{J\hbar^2 S}{2} \sum_m (a_{m+1}^\dagger - a_m^\dagger)(a_{m+1} - a_m) + O(S^0) \]

- Taking continuum limit, \( a_{m+1} - a_m \simeq \partial_x a(x)|_{x=m} \) (unit spacing),

\[ \hat{H} = -JN\hbar^2 S^2 + \frac{J\hbar^2 S}{2} \int_0^N dx (\partial_x a^\dagger)(\partial_x a) + O(S^0) \]

- As with harmonic chain, Hamiltonian can be diagonalized by Fourier transformation. With periodic boundary conditions, \( a_{m+N}^\dagger = a_m^\dagger \),

\[ a(x) = \frac{1}{\sqrt{N}} \sum_k e^{ikx} a_k, \quad a_k = \frac{1}{\sqrt{N}} \int_0^N dx e^{-ikx} a(x) \]

where sum on \( k = 2\pi n/N \), runs over integers \( n \) and \([a_k, a_{k'}^\dagger] = \delta_{kk'}\),

\[ \int_0^N dx (\partial_x a^\dagger)(\partial_x a) = \sum_{kk'} (-ika_k^\dagger)(ik' a_{k'}) \frac{1}{N} \int_0^N dx e^{i(k-k')x} = \sum_k k^2 a_k^\dagger a_k \]

\[ \delta_{kk'} \]
Spin wave theory

As a result, we obtain

\[ \hat{H} \simeq -JN\hbar^2 S^2 + \sum_k \hbar \omega_k a_k^{\dagger} a_k \]

where \( \omega_k = J\hbar Sk^2 \) represents the dispersion of the spin excitations (cf. linear dispersion of harmonic chain).

As with harmonic chain, magnetic system defined by massless low-energy collective excitations known as spin waves or magnons.

Spin wave spectrum can be recorded by neutron scattering measurements.