Lecture 16

Quantum field theory: from phonons to photons

Field theory: from phonons to photons

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- 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.

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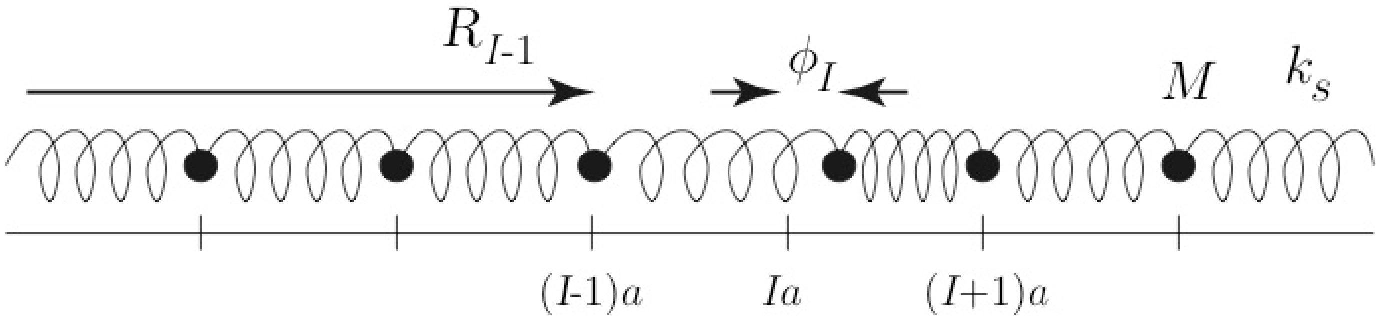
Atomic chain

- 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).



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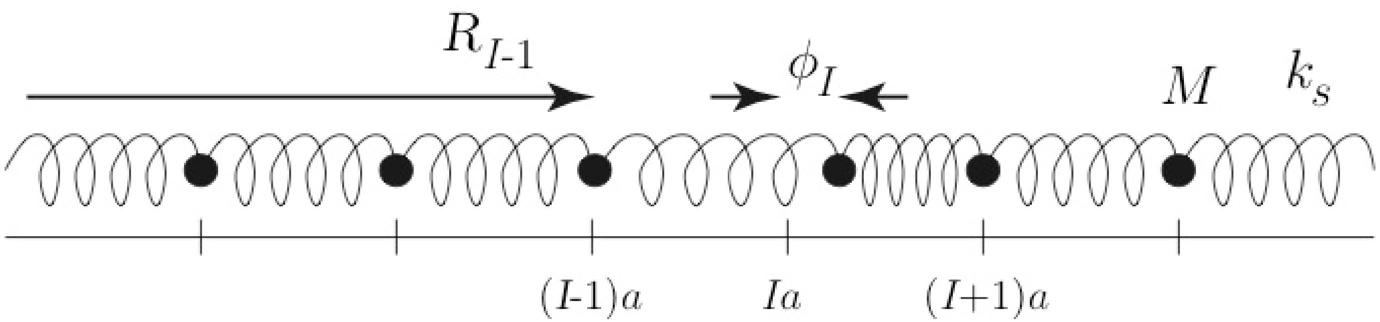

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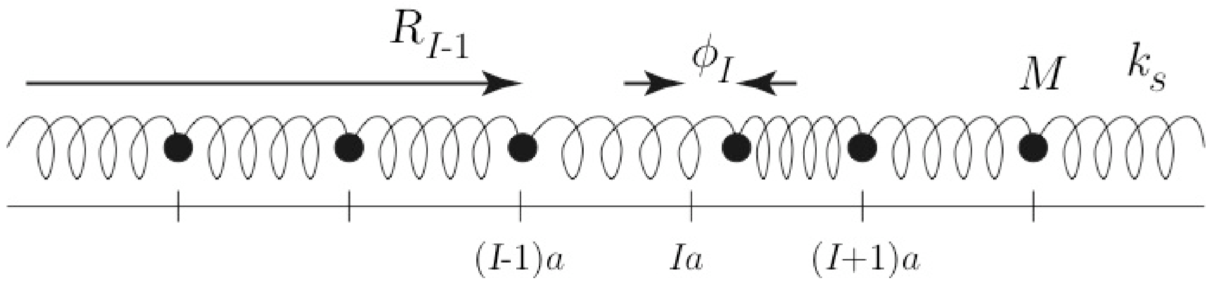
Classical chain



- For an N-atom chain, with periodic boundary conditions: $x_{N+1} = Na + x_1$, the Lagrangian is given by,

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

- 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 ϕ_n is displacement from equlibrium,

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

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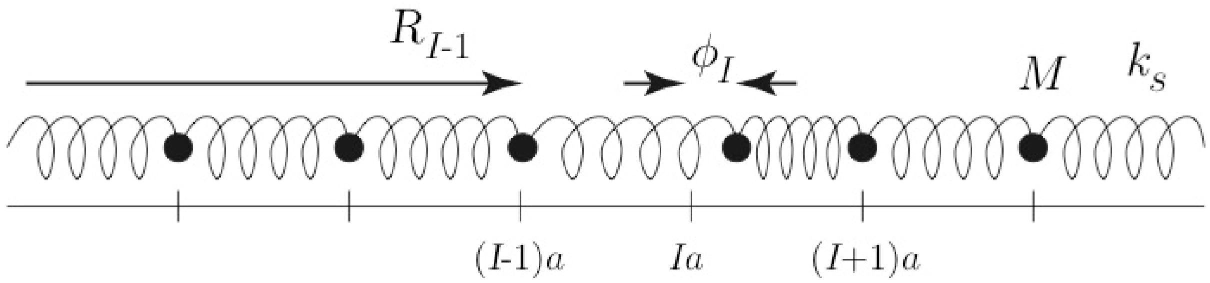

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Classical chain: equations of motion

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- 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

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

  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

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- 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 $\partial_{\dot{\phi}_n} L = m\dot{\phi}_n$ 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,

$$m\ddot{\phi}_n = -k_s(\phi_n - \phi_{n+1}) - k_s(\phi_n - \phi_{n-1}) \qquad \text{for each } n$$

- 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

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

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- 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

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

- We therefore find that

$$\boxed{\omega = \omega_k = \sqrt{\frac{2k_s}{m}(1 - \cos(ka))} = 2\sqrt{\frac{k_s}{m}}|\sin(ka/2)|}$$

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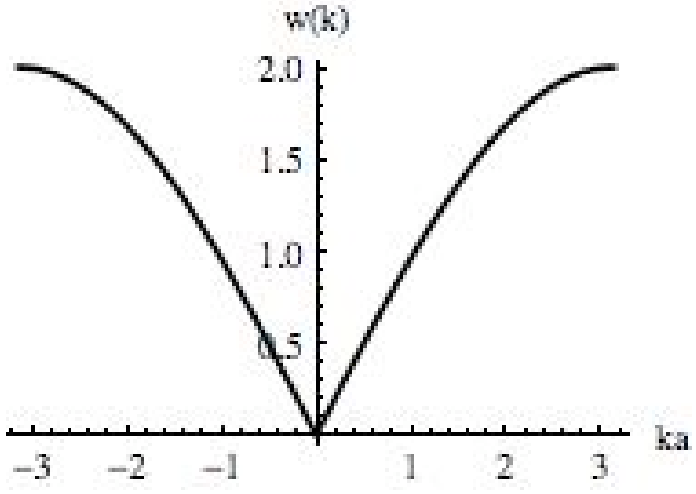

- At low energies, $k \to 0$, (i.e. long wavelengths) the **linear** dispersion relation,

$$\boxed{\omega_k \simeq v|k|}$$

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.

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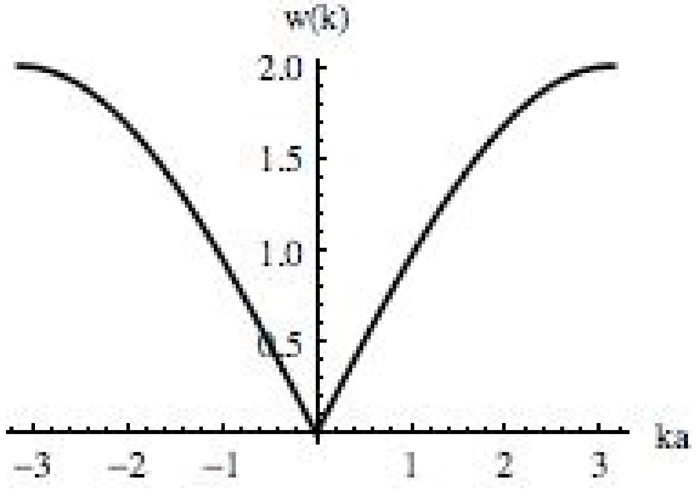

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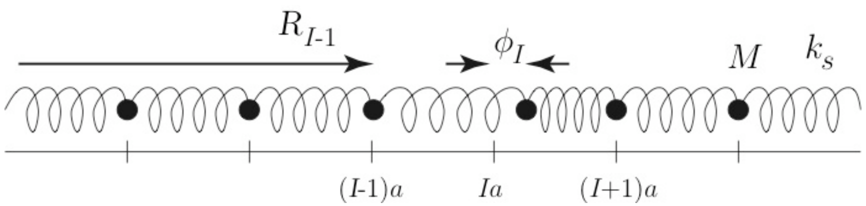

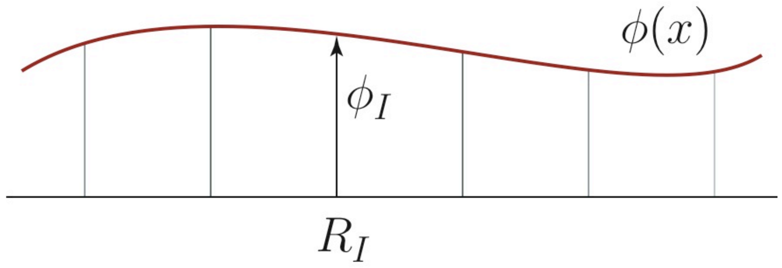

- For low energy dynamics, relative displacement of neighbours is small, $|\phi_{n+1} - \phi_n| \ll a$, and we can transfer to a continuum limit:

$$\phi_n \to \phi(x)|_{x=na}, \quad \phi_{n+1} - \phi_n \to a\partial_x \phi(x)|_{x=na}, \quad \sum_{n=1}^{N} \to \frac{1}{a}\int_0^{L=Na} dx$$

- Lagrangian $L[\phi] = \int_0^L dx\, \mathcal{L}(\dot{\phi}, \phi)$, where **Lagrangian density**

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

$\rho = m/a$ is mass per unit length and $\kappa_s = k_s/a$.

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- 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 **(classical) field**.
- Dynamics of $\phi(x, t)$ specified by the Lagrangian and action functional

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

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Dynamics of harmonic chain

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

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

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

- Integrating by parts

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

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

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

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- 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.

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Quantization of classical chain

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

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

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

1. Define canonical momentum: $p = \partial_{\dot{x}} \mathcal{L}(\dot{x}, x)$
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: $[\hat{p}, \hat{x}] = -i\hbar$

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

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

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Quantization of classical chain

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

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

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

and the canonical commutation relations,

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

Quantum chain

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

- 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:

$$\left\{ \begin{array}{c} \hat{\phi}(x) \\ \hat{\pi}(x) \end{array} \right. = \frac{1}{L^{1/2}} \sum_k e^{\{\pm ikx} \left\{ \begin{array}{c} \hat{\phi}_k \\ \hat{\pi}_k \end{array} \right. , \quad \left\{ \begin{array}{c} \hat{\phi}_k \\ \hat{\pi}_k \end{array} \right. = \frac{1}{L^{1/2}} \int_0^L dx\; e^{\{\mp ikx} \left\{ \begin{array}{c} \hat{\phi}(x) \\ \hat{\pi}(x) \end{array} \right.$$

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

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

- Operator-valued functions, $\hat{\phi}$ and $\hat{\pi}$, referred to as **quantum fields**.
- Hamiltonian represents a *formulation* but not yet a *solution*.
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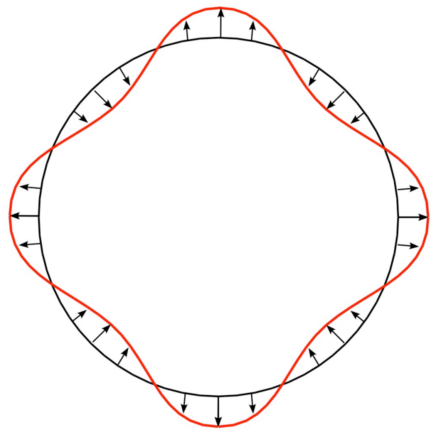
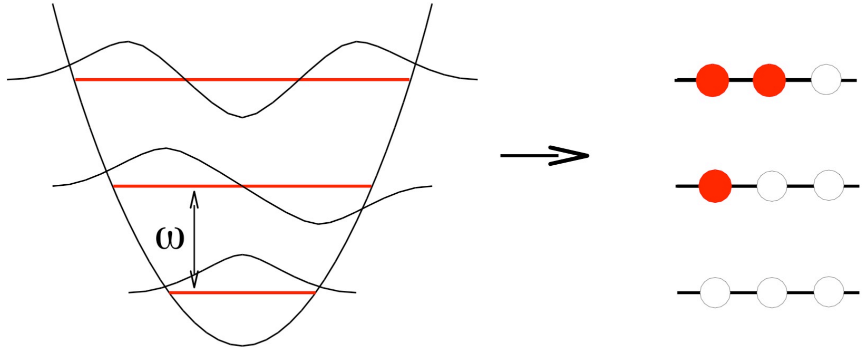


- Hamiltonian describes set of independent quantum harmonic oscillators (existence of indicies k and $-k$ is not crucial).
- Interpretation: classically, chain supports discrete set of wave-like excitations, each indexed by wavenumber $k = 2\pi m/L$.
- In quantum picture, each of these excitations described by an oscillator Hamiltonian operator with a k-dependent frequency.
- Each oscillator mode involves all $N \to \infty$ microscropic degrees of freedom – it is a **collective excitation** of the system.

Quantum harmonic oscillator: revisited

$$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 x^2}$$



- 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!

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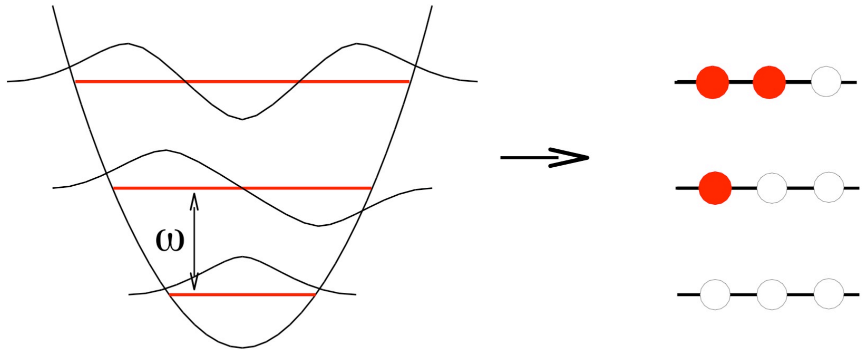

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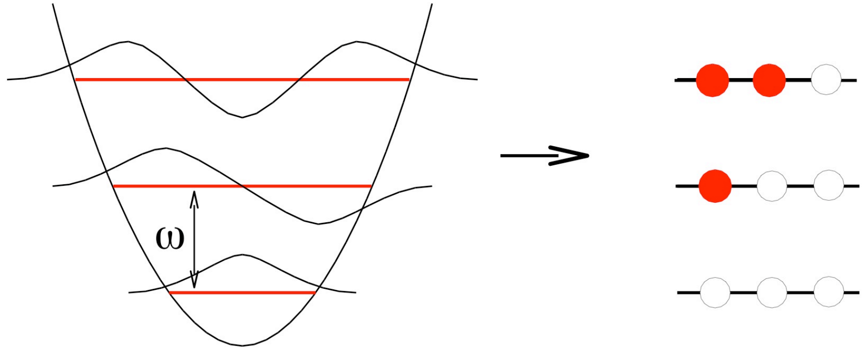

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$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + i \frac{\hat{p}}{m\omega} \right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - i \frac{\hat{p}}{m\omega} \right)$$

which fulfil the commutation relations $[a, a^\dagger] = 1$, we have,

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

- 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.

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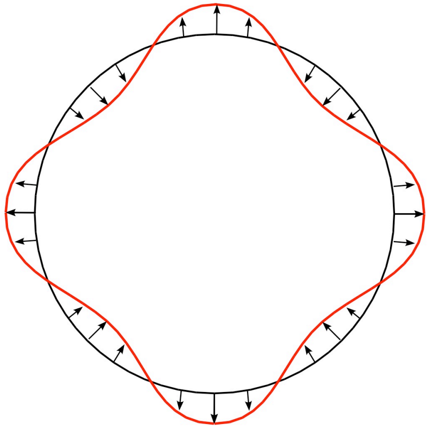
$$\boxed{\hat{H} = \sum_k \left[\frac{1}{2\rho} \hat{\pi}_k \hat{\pi}_{-k} + \frac{1}{2} \rho \omega_k^2 \hat{\phi}_k \hat{\phi}_{-k} \right]}$$



- Inspired by ladder operator formalism for harmonic oscillator, set

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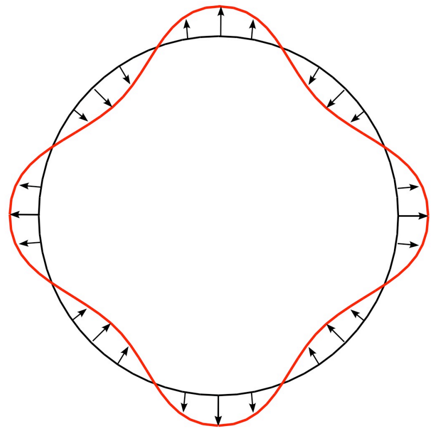

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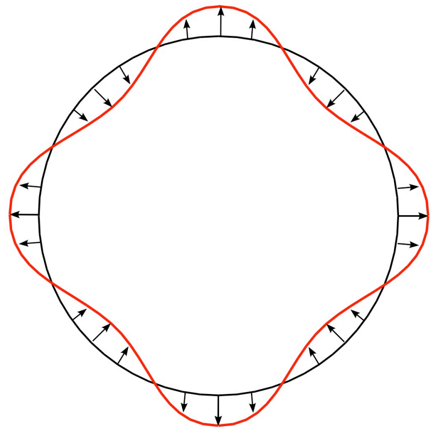

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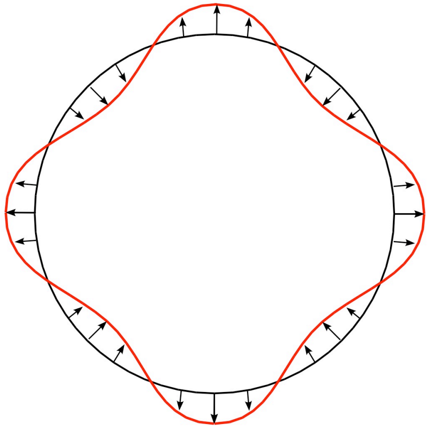

- Low energy excitations of discrete atomic chain behave as discrete particles (even though they describe the collective motion of an infinite number of "fundamental" degrees of freedom) describing oscillator wave-like modes.
- These particle-like excitations, known as **phonons**, are characterised by wavevector k and have a linear dispersion, $\omega_k = v|k|$.
- A generic state of the system is then given by

$$\boxed{|\{n_k\}\rangle = \frac{1}{\sqrt{\prod_i n_i!}} (a_{k_1}^\dagger)^{n_1} (a_{k_2}^\dagger)^{n_2} \cdots |0\rangle}$$

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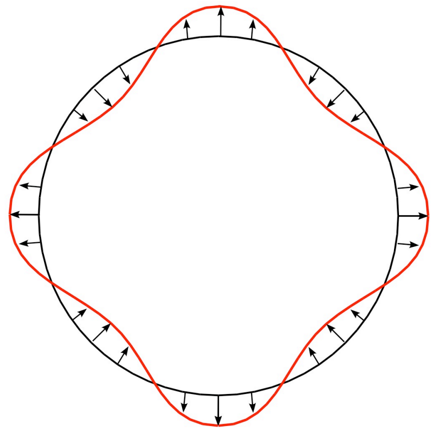

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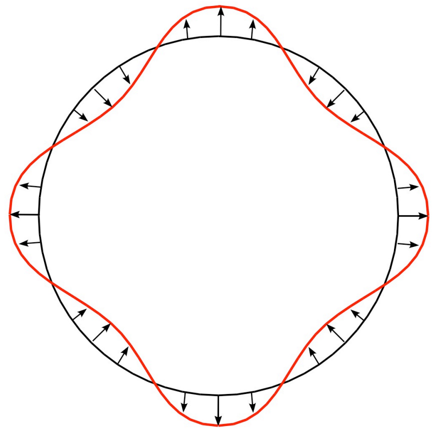

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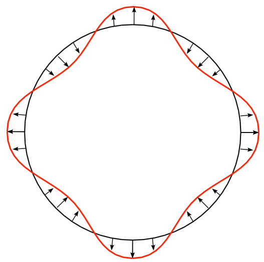

- In principle, we could now retrace our steps and express the elementary excitations, $a_k^\dagger|0\rangle$, in terms of the continuum fields, $\phi(x)$ (or even the discrete degrees of freedom ϕ_n). **But why should we?**
- Phonon excitations represent perfectly legitimate (bosonic) particles which have physical manifestations which can be measured directly.
- We can regard phonons are “fundamental” and abandon microscopic degrees of freedom as being irrelevant on low energy scales!
- This heirarchy 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.

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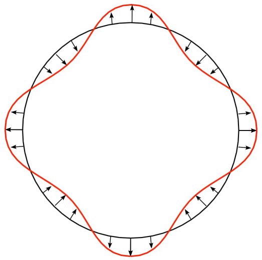

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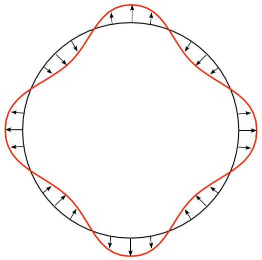

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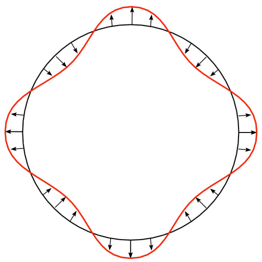

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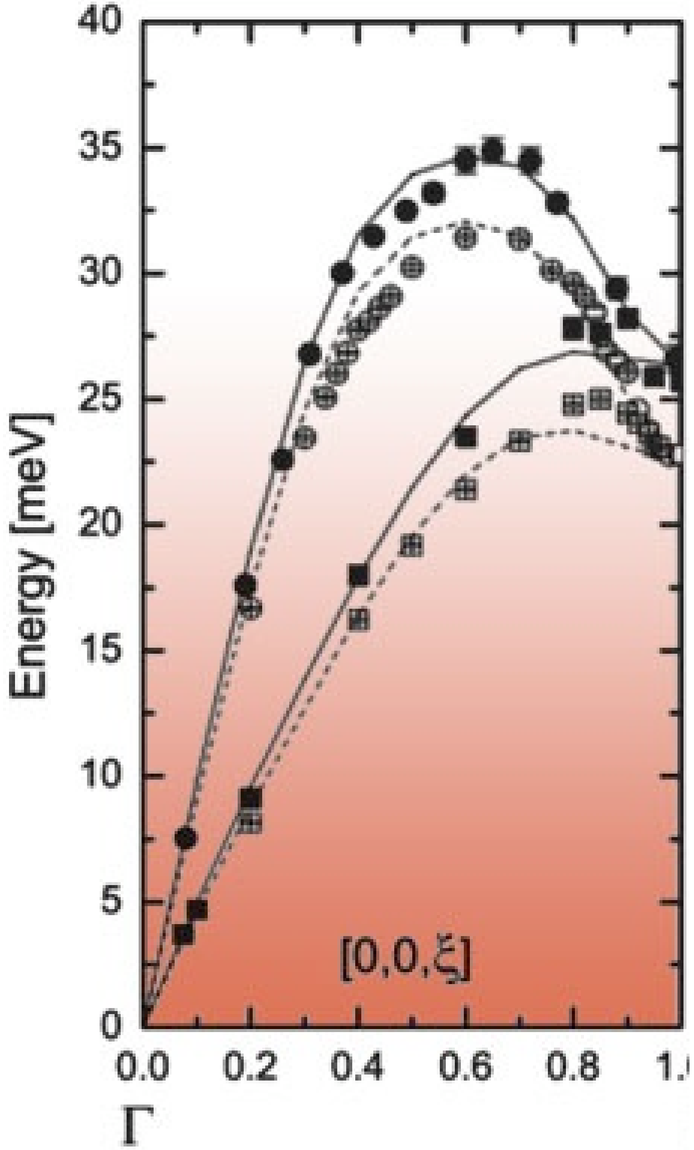
$$\boxed{\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right), \qquad \omega_k = v|k|}$$

- **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**.



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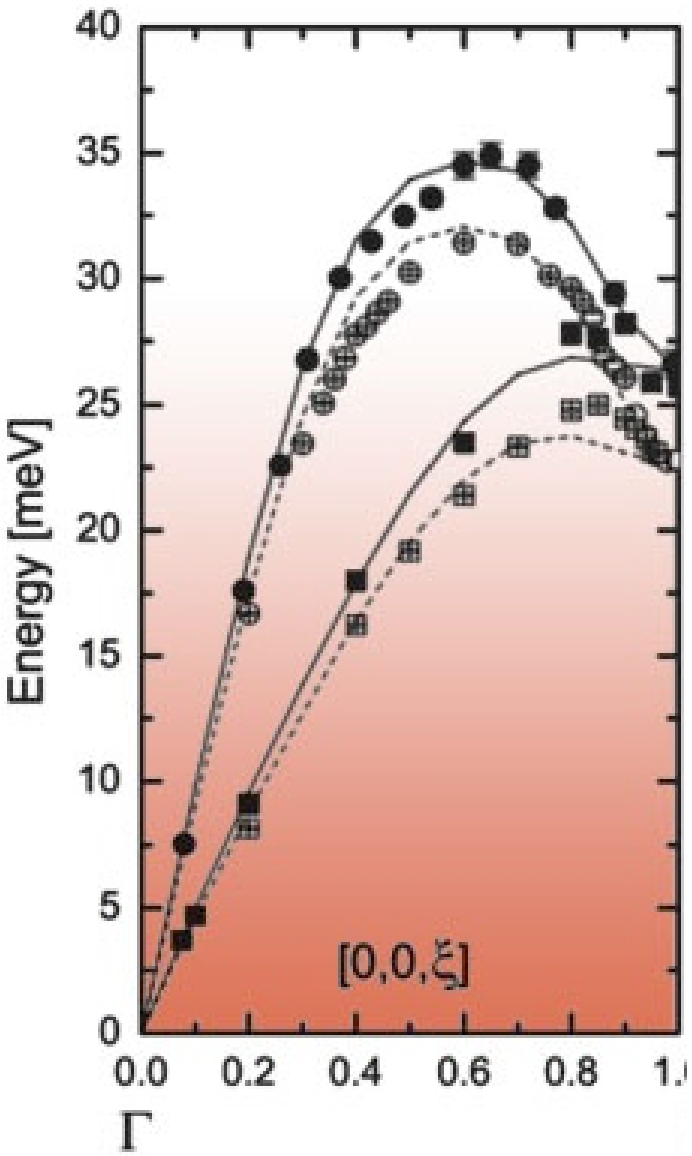
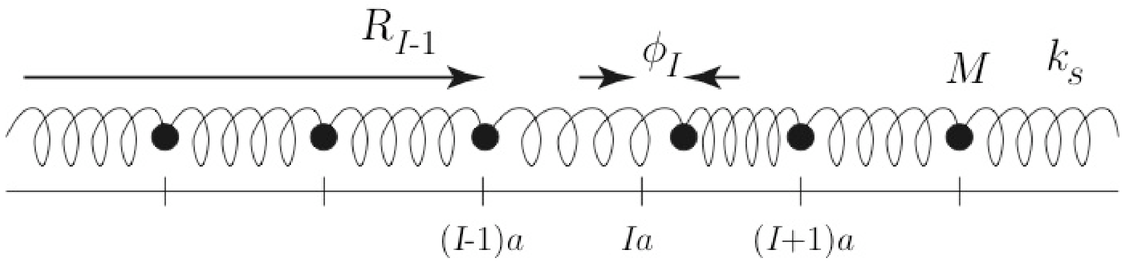


Quantization of the harmonic chain: recap



- Starting with the classical Lagrangian for a harmonic chain,

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

  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

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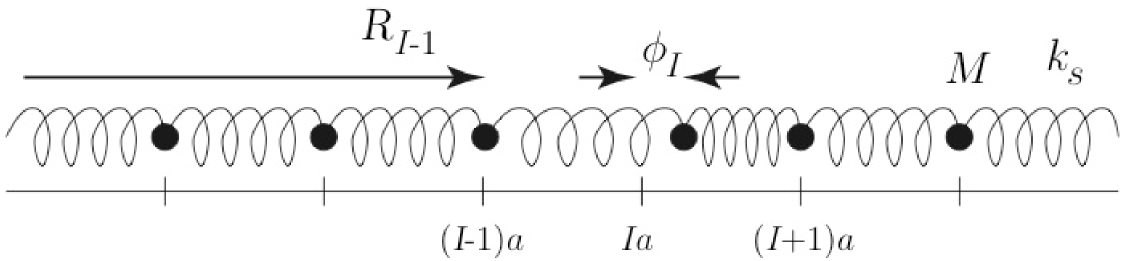
Quantization of the harmonic chain: recap



- Starting with the classical Lagrangian for a harmonic chain,

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

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Quantization of harmonic chain: recap

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

$$\boxed{\rho \ddot{\phi} = \kappa_s a^2 \partial_x^2 \phi}$$

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:

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

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

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

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

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

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

$$\left\{ \begin{array}{c} \hat{\phi}(x) \\ \hat{\pi}(x) \end{array} \right. = \frac{1}{L^{1/2}} \sum_k e^{\{\pm ikx} \left\{ \begin{array}{c} \hat{\phi}_k \\ \hat{\pi}_k \end{array} \right.$$

with $k = 2\pi m/L$, m integer, whereupon the Hamiltonian takes the "near-diagonal" form,

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

Quantization of harmonic chain: recap

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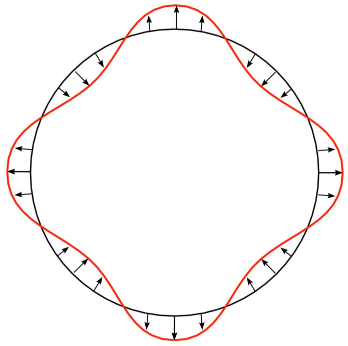

- $\hat{H}$ describes set of independent oscillators with k-dependent frequency. Each mode involves all $N \to \infty$ microscropic degrees of freedom – it is a **collective excitation**.
- Inspired by ladder operator formalism, setting

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

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

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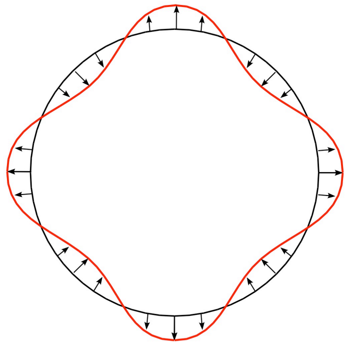

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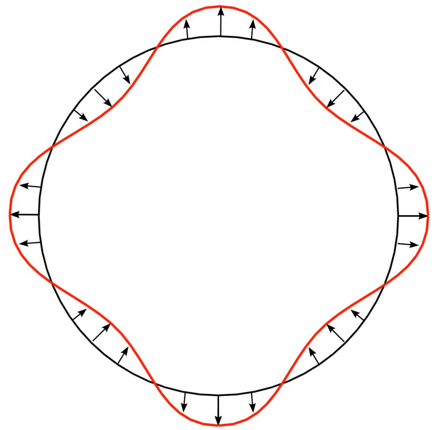

- Low energy excitations of discrete atomic chain behave as discrete particles (even though they describe collective motion of an infinite number of "fundamental" degrees of freedom).
- These particle-like excitations, known as **phonons**, are characterised by wavevector k and have a linear dispersion, $\omega_k = v|k|$.
- A generic state of the system is then given by

$$\boxed{|\{n_k\}\rangle = \frac{1}{\sqrt{\prod_i n_i!}} (a_{k_1}^\dagger)^{n_1} (a_{k_2}^\dagger)^{n_2} \cdots |0\rangle}$$

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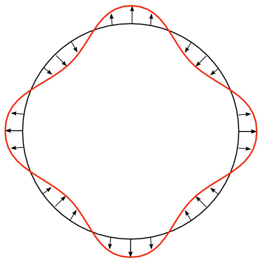

- In theory, we could now retrace our steps and express the elementary excitations, $a_k^\dagger|0\rangle$, in terms of continuum fields, $\phi(x)$ (or even the discrete degrees of freedom ϕ_n). **But why should we?**
- Phonon excitations represent perfectly "legitimate" particles which have physical 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!)

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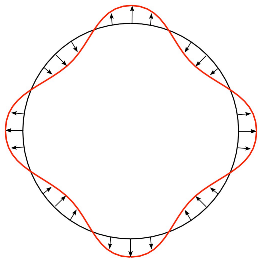

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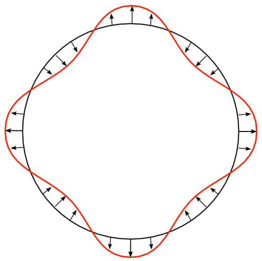

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Quantization of harmonic chain: second quantization

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,

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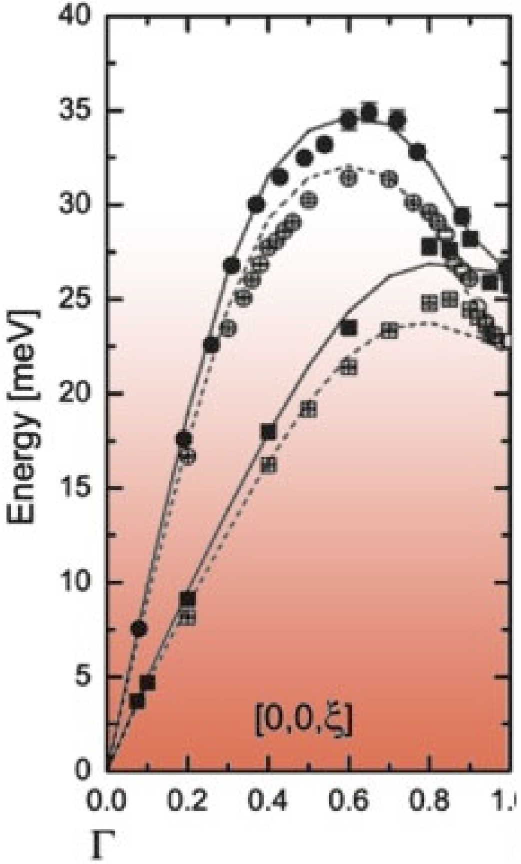
Quantization of harmonic chain: further lessons

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

- **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**.



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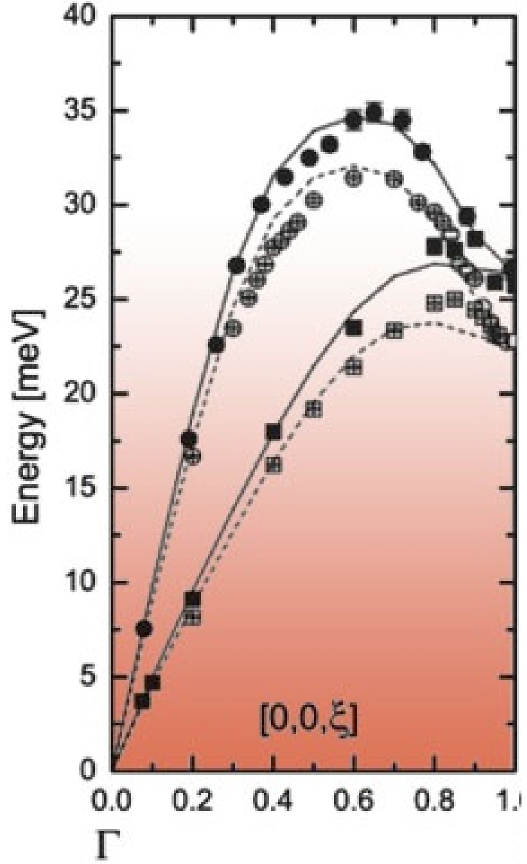
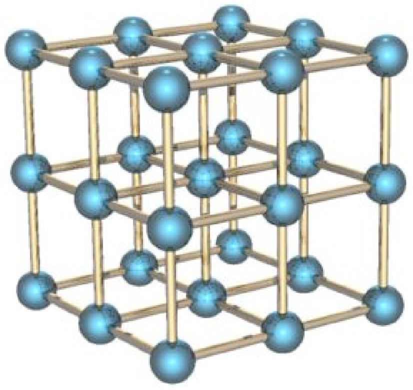


Three-dimensional lattices



- Our analysis focussed on longitudinal vibrations of one-dimensional chain. In three-dimensions, each mode associated with three possible polarizations, λ: two transverse and one longitudinal.
- Taking into account all polarizations

$$\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}\lambda} \left(a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + \frac{1}{2} \right)$$

where $\omega_{\mathbf{k}\lambda} = v_\lambda |\mathbf{k}|$ and v_λ are respective sound wave velocities.
- Let us apply this result to obtain internal energy and specific heat due to phonons.

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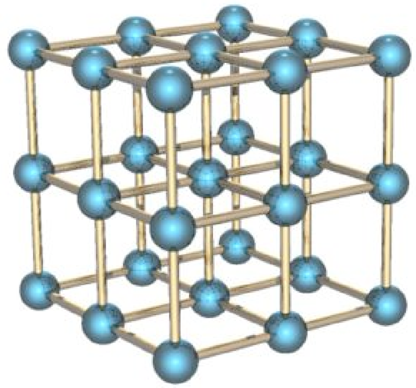

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Example: Debye theory of solids

- For equilibrium distribution, average phonon occupancy of state $(\mathbf{k}, \lambda)$ given by Bose-Einstein distribution, $n_{\rm B}(\hbar\omega_{\mathbf{k}}) \equiv \frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_{\rm B}T}-1}$.
- The internal energy therefore given by

$$E = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left[\frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_{\rm B}T} - 1} + \frac{1}{2}\right]$$

- In thermodynamic limit, $\sum_{\mathbf{k}} \to \frac{L^3}{(2\pi)^3} \int_0^{k_{\rm D}} d^3k = \frac{L^3}{2\pi^2} \int_0^{k_{\rm D}} k^2\, dk$, with cut-off $k_{\rm D}$ fixed by ensuring that total number of modes matches degrees of freedom, $\frac{1}{(2\pi/L)^3} \frac{4}{3}\pi k_{\rm D}^3 = N \equiv \frac{L^3}{a^3}$, i.e. $k_{\rm D}^3 = \frac{6\pi^2}{a^3}$
- Dropping zero point fluctuations, if $v_\lambda = v$ (independent of λ), internal energy/particle given by

$$\varepsilon \equiv \frac{E}{N} = 3 \times \frac{a^3}{2\pi^2} \int_0^{k_{\rm D}} k^2\, dk\, \frac{\hbar v k}{e^{\hbar v k/k_{\rm B}T} - 1}$$

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- Defining Debye temperature, $k_{\mathrm{B}} T_{\mathrm{D}} = \hbar v k_{\mathrm{D}}$,

$$\boxed{\varepsilon = 9 k_{\mathrm{B}} T \left(\frac{T}{T_{\mathrm{D}}} \right)^3 \int_0^{T_{\mathrm{D}}/T} \frac{z^3\, dz}{e^z - 1}}$$

- Leads to specific heat per particle,

$$\boxed{c_V = \partial_T \varepsilon = 9 k_{\mathrm{B}} \left(\frac{T}{T_{\mathrm{D}}} \right)^3 \int_0^{T_{\mathrm{D}}/T} \frac{z^4\, dz}{(e^z - 1)^2} = \begin{cases} 3 k_{\mathrm{B}} & T \gg T_{\mathrm{D}} \\ A T^3 & T \ll T_{\mathrm{D}} \end{cases}}$$

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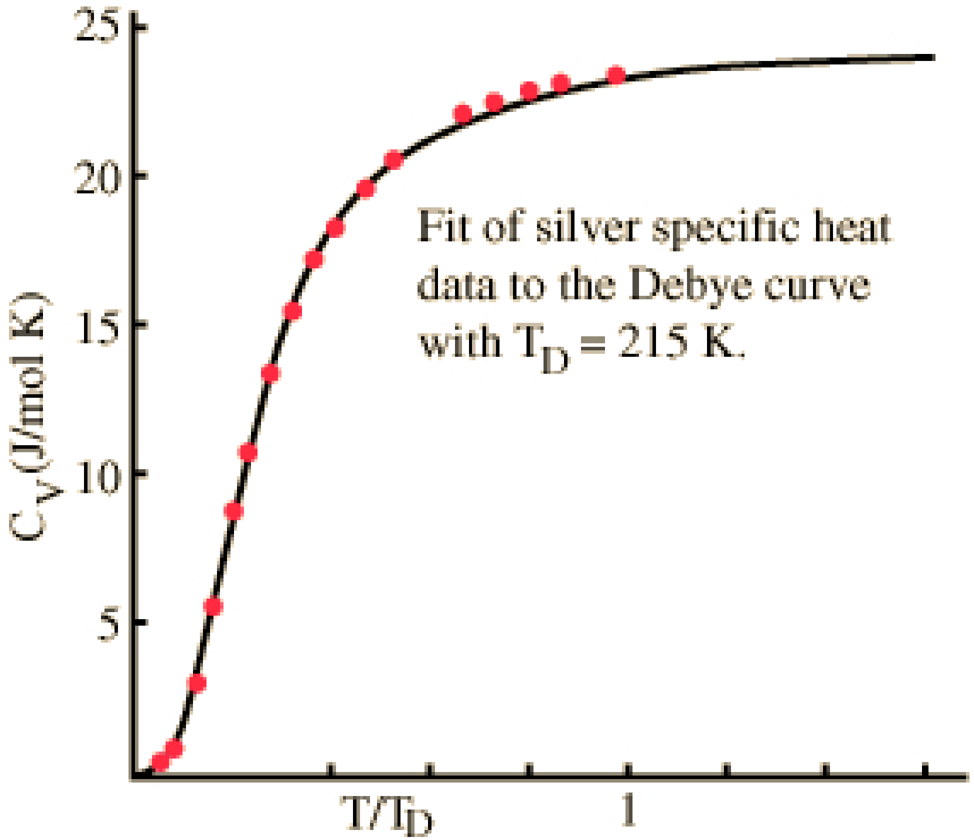

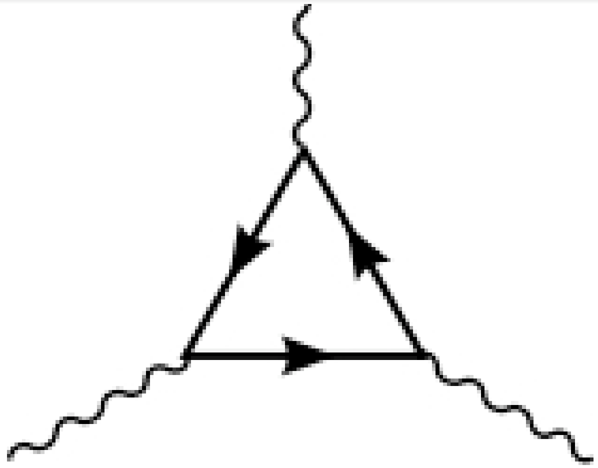

Lecture 17

Quantization of the Electromagnetic Field

Quantum electrodynamics

- As with harmonic chain, electromagnetic (EM) field satisfies wave equation in vacua.

$$\frac{1}{c^2}\ddot{\mathbf{E}} = \nabla^2\mathbf{E}, \qquad \frac{1}{c^2}\ddot{\mathbf{B}} = \nabla^2\mathbf{B}$$

- 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.

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Classical theory of electromagnetic field

- In vacuum, Lagrangian density of EM field given by

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

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

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

- Corresponding classical equations of motion lead to wave equation

$$\frac{1}{c^2} \ddot{\mathbf{A}} = \nabla^2 \mathbf{A} \qquad \longleftrightarrow \qquad \partial_\mu F^{\mu\nu} = 0$$

Classical theory of electromagnetic field

- In vacuum, Lagrangian density of EM field given by

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

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.

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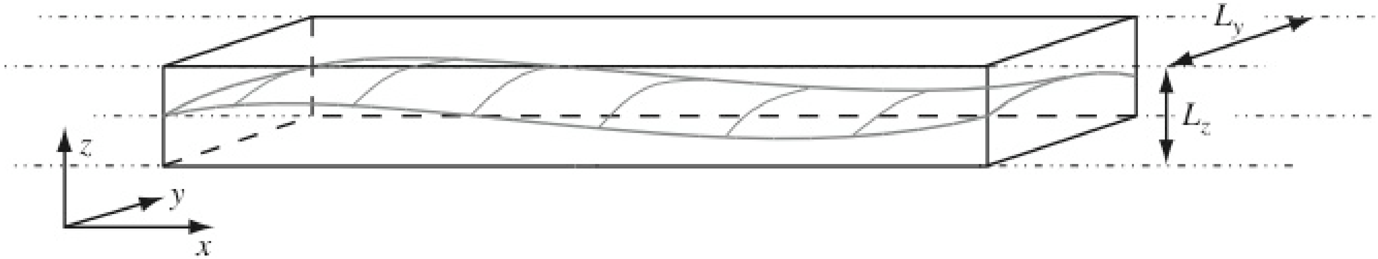
Classical theory of EM field: waveguide

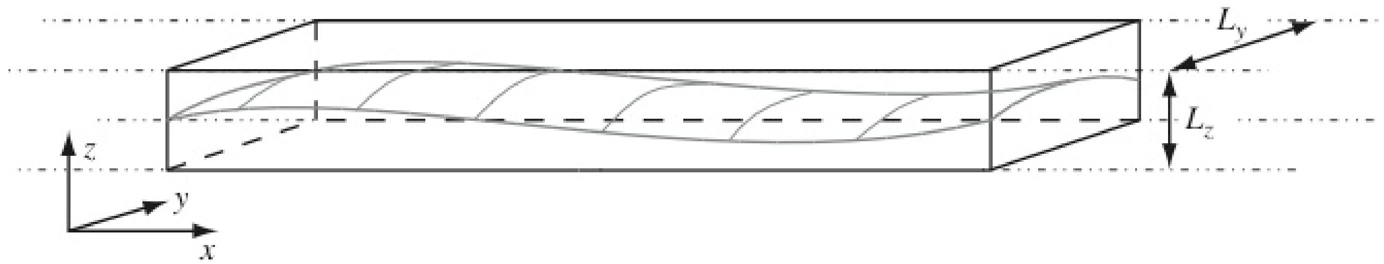
$$\boxed{L[\dot{\mathbf{A}}, \mathbf{A}] = \frac{1}{2\mu_0} \int d^3x \left[\frac{1}{c^2} \dot{\mathbf{A}}^2 - (\nabla \times \mathbf{A})^2 \right]}$$

- We can circumvent difficulties by considering simplifed 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, $\hat{\mathbf{e}}_n \times \mathbf{E} \equiv \mathbf{E}_{||}|_{\text{boundary}} = 0$ and $\hat{\mathbf{e}}_n \cdot \mathbf{B} \equiv \mathbf{B}_{\perp}|_{\text{boundary}} = 0$.

Classical theory of EM field: waveguide



- For waveguide, general vector potential configuration may be expanded in eigenmodes of classical wave equation,

$$\boxed{-\nabla^2 \mathbf{u}_k(\mathbf{x}) = \lambda_k \mathbf{u}_k(\mathbf{x})}$$

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

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

$$\mathbf{u}_k = \frac{2}{\sqrt{V}} \sin(\pi y/L_y) \sin(kx)\, \hat{\mathbf{e}}_z, \qquad \lambda_k = k^2 + \left(\frac{\pi}{L_y}\right)^2$$

Classical theory of EM field: waveguide

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

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

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

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

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

Quantization of classical EM field

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1. Define canonical momenta $\pi_k = \partial_{\dot{\alpha}_k} \mathcal{L} = \epsilon_0 \dot{\alpha}_k$, 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 $\pi_k \to \hat{\pi}_k$.
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- Following analysis of atomic chain, if we introduce ladder operators,

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

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

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

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

Quantization of EM field: remarks

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

- Elementary particle-like excitations of EM field, known as **photons**, are created an annihilated by operators $a_k^\dagger$ and a_k.

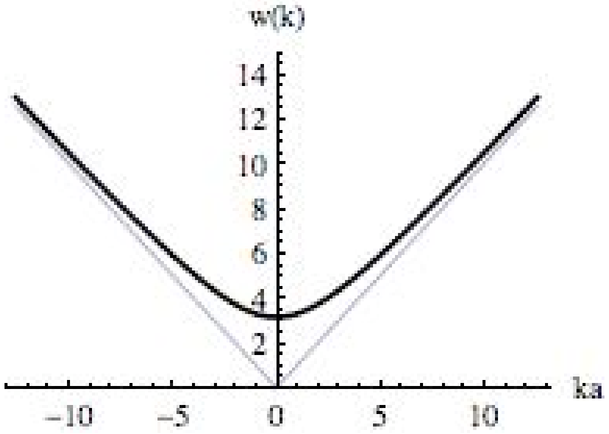
$$a_k^\dagger|n_k\rangle = \sqrt{n_k+1}|n_k+1\rangle, \qquad a_k|n_k\rangle = \sqrt{n_k}|n_k-1\rangle$$

- 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,

$$\boxed{\omega_k \simeq c|k|}$$



Quantization of EM field: generalization

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 $\hat{\mathbf{A}}(\mathbf{x}) = \sum_k \hat{\alpha}_k \mathbf{u}_k$ where

$$\boxed{\hat{\alpha}_k = \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}}(a_k + a_k^\dagger)}$$

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

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

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

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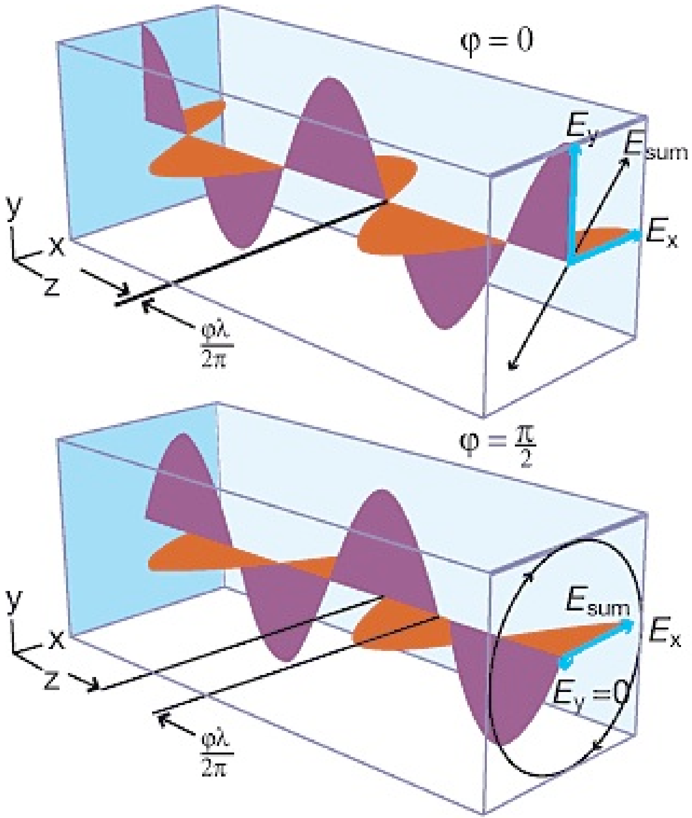

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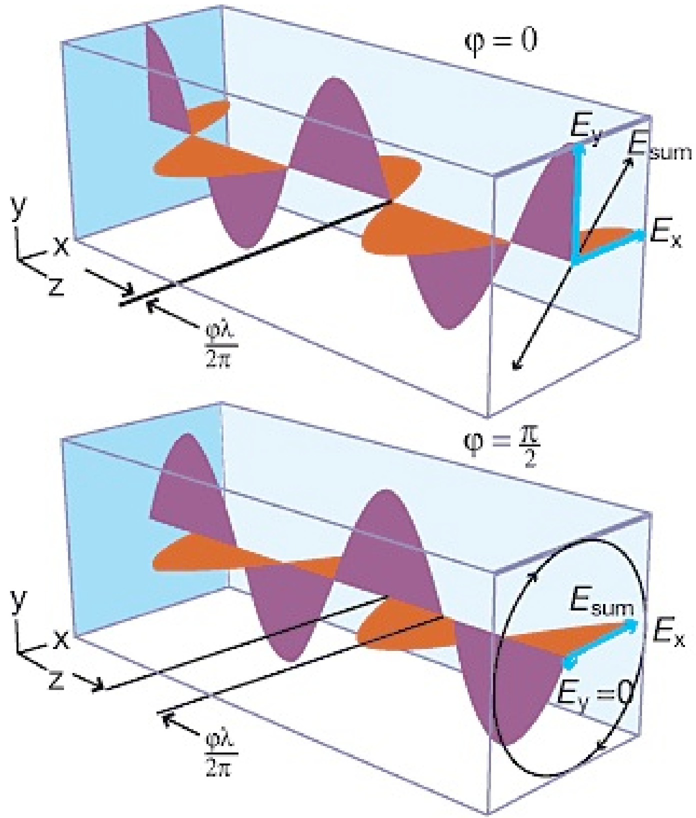

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- With these definitions, the photon Hamiltonian then takes the form

$$\boxed{\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left[a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} + 1/2\right]}$$

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

$$\boxed{|\{n_{\mathbf{k}\lambda}\}\rangle = \frac{1}{\sqrt{\prod_{\mathbf{k}\lambda} n_{\mathbf{k}\lambda}!}} (a^\dagger_{\mathbf{k}_1\lambda})^{n_{\mathbf{k}_1\lambda}} (a^\dagger_{\mathbf{k}_2\lambda})^{n_{\mathbf{k}_2\lambda}} \cdots |\Omega\rangle}$$

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, $\mathbf{S}/c^2$ where $\mathbf{S} = \mathbf{E} \times \mathbf{B}/\mu_0$ denotes **Poynting vector**, i.e. total **momentum**

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

- After quantization, find (exercise)

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Angular momentum carried by photon field

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

$$\mathbf{M} = -\int d^3x\, \dot{\mathbf{A}} \times \mathbf{A} \mapsto \hat{\mathbf{M}} = -i\hbar \sum_{\mathbf{k}} \hat{\mathbf{e}}_{\mathbf{k}} \left[a^\dagger_{\mathbf{k}1} a_{\mathbf{k}2} - a^\dagger_{\mathbf{k}2} a_{\mathbf{k}1} \right]$$

- Defining creation operators for right/left circular polarization,

$$a^\dagger_{\mathbf{k}\mathrm{R}} = \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}1} + i a^\dagger_{\mathbf{k}2}), \qquad a^\dagger_{\mathbf{k}\mathrm{L}} = \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}1} - i a^\dagger_{\mathbf{k}2})$$

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

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Casimir effect

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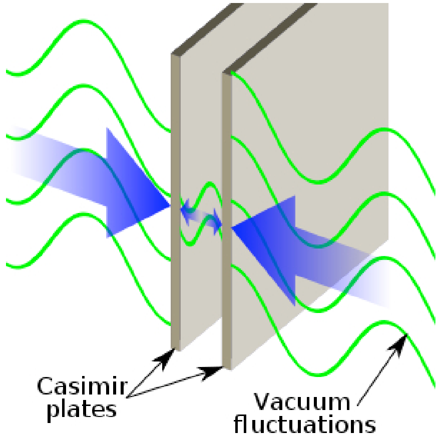


- As with harmonic chain, quantization of EM field $\rightsquigarrow$ zero-point fluctuations with physical manifestations.
  - Consider two metallic plates, area A, separated by distance d – quantization of EM field leads to vacuum energy/unit area

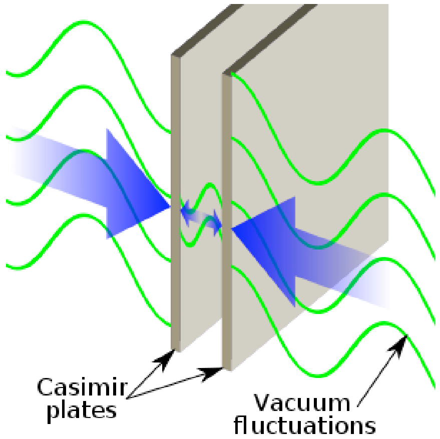
$$\frac{\langle E \rangle}{A} = 2 \times \int \frac{d^2 k_\perp}{(2\pi)^2} \sum_{n=1}^{\infty} \frac{\hbar\omega_{\mathbf{k}_\perp n}}{2} = -\frac{\pi^2}{720}\frac{\hbar c}{d^3}, \quad \omega_{\mathbf{k}_\perp n} = c\sqrt{\mathbf{k}_\perp^2 + \frac{(\pi n)^2}{d^2}}$$

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

$$\boxed{\frac{F_C}{A} = -\frac{\partial_d \langle E \rangle}{A} = -\frac{\pi^2}{240}\frac{\hbar c}{d^4}}$$

Casimir effect

$$\boxed{\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left[a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} + 1/2\right]}$$



- As with harmonic chain, quantization of EM field $\rightsquigarrow$ 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

$$\frac{\langle E \rangle}{A} = 2 \times \int \frac{d^2 k_\perp}{(2\pi)^2} \sum_{n=1}^{\infty} \frac{\hbar\omega_{\mathbf{k}_\perp n}}{2} = -\frac{\pi^2}{720} \frac{\hbar c}{d^3}, \qquad \omega_{\mathbf{k}_\perp n} = c\sqrt{\mathbf{k}_\perp^2 + \frac{(\pi n)^2}{d^2}}$$

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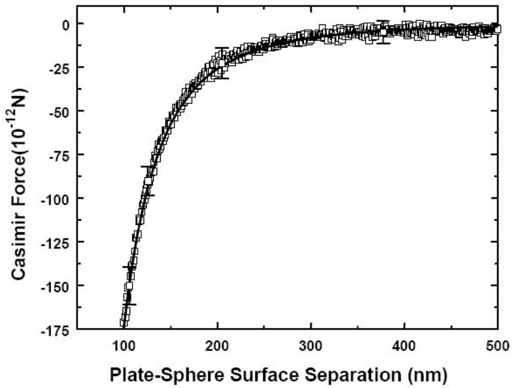


Quantum field theory: summary

- Starting with continuum field theory of the classical harmonic chain,

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

  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**,

$$\boxed{\hat{H} = \sum_k \hbar\omega_k (a_k^\dagger a_k + 1/2), \qquad \hbar\omega_k = v|k|}$$

- In three-dimensional system, modes acquire polarization index, λ.

Quantum field theory: summary

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

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

we applied quantization procedure to establish quantum theory.

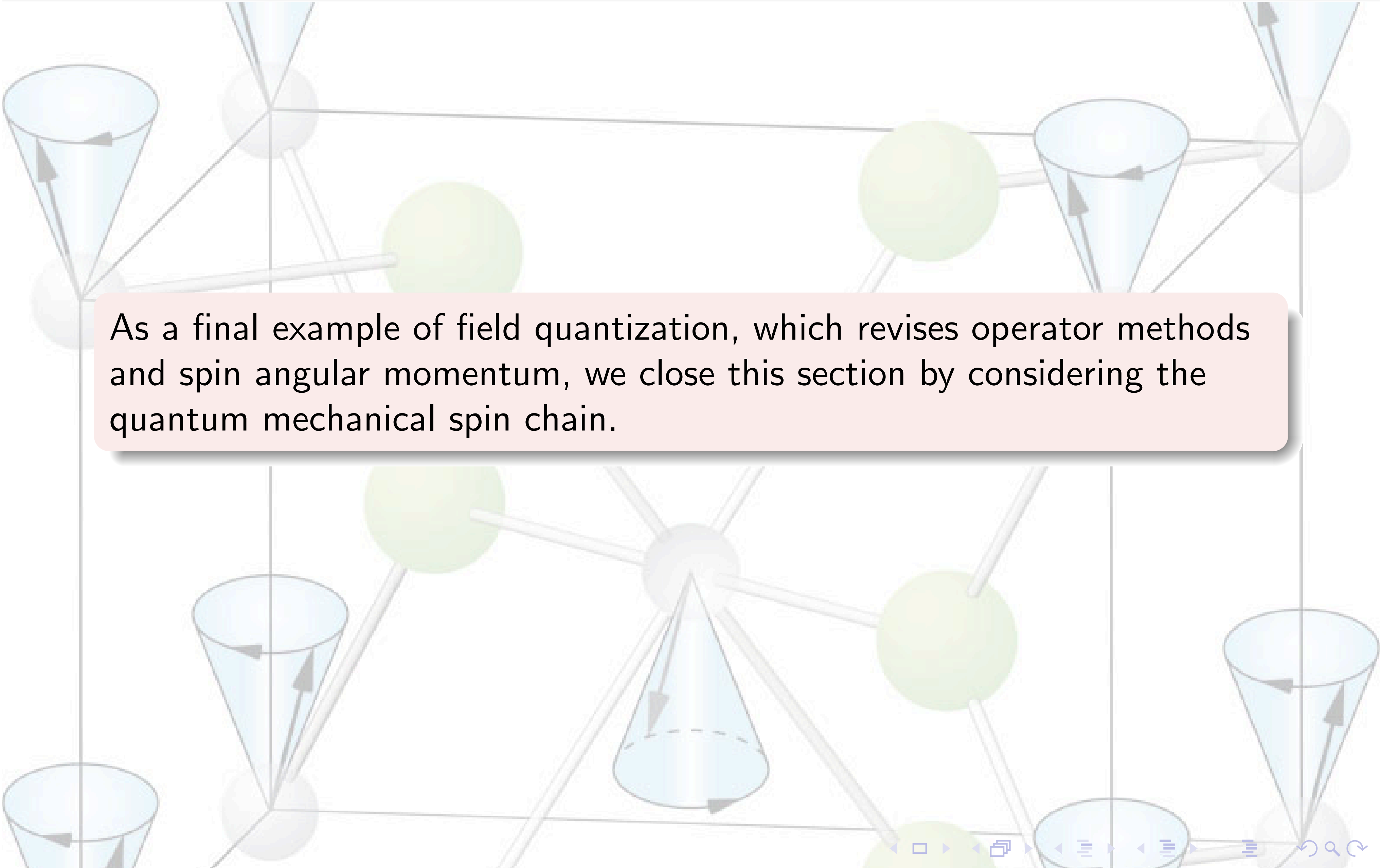
- These studies show that low-energy excitations of EM field described by (bosonic) particle-like modes known as **photons**,

$$\boxed{\hat{H} = \sum_k \hbar\omega_k (a_k^\dagger a_k + 1/2), \qquad \omega_k = c(k^2 + (\pi/L_y)^2)^{1/2}}$$

- In three-dimensional system modes acquire polarization index, λ.

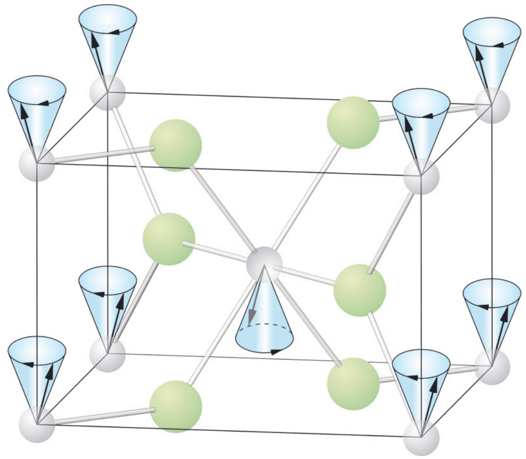
$$\boxed{\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} (a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + 1/2), \qquad \omega_{\mathbf{k}} = c|\mathbf{k}|}$$

Spin wave theory



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.

Spin wave theory



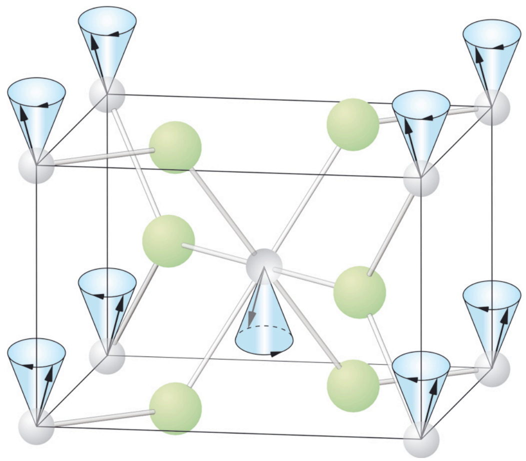
- In correlated electron systems Coulomb interaction can result in electrons becoming localized – the **Mott transition**.
- However, in these insulating materials, the spin degrees of freedom carried by the constituent electrons can remain mobile – such systems are described by quantum magnetic models,

$$\boxed{\hat{H} = \sum_{m \neq n} J_{mn} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n}$$

where **exchange couplings** J_{mn} denote matrix elements coupling local moments at lattice sites m and n.

Spin wave theory

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



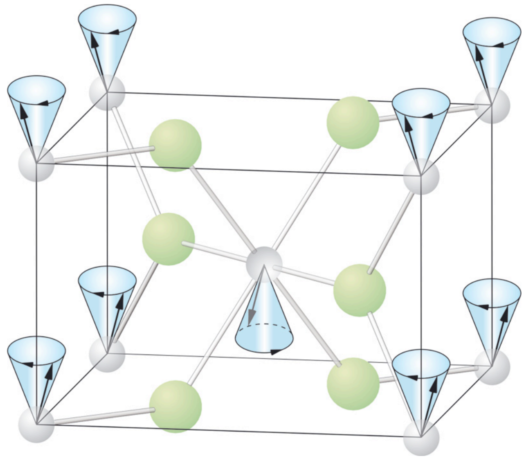
- Since matrix elements J_{mn} decay rapidly with distance, we may restrict attention to just neighbouring sites, $J_{mn} = J\delta_{m,n\pm 1}$.
- Although J typically positive (leading to **antiferromagnetic** coupling), here we consider them negative leading to **ferromagnetism** – i.e. neighbouring spins want to lie parallel.
- Consider then the 1d **spin S quantum Heisenberg ferromagnet**,

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

where $J > 0$, and spins obey spin algebra, $[\hat{S}^\alpha_m, \hat{S}^\beta_n] = i\hbar\delta_{mn}\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma_m$.

Spin wave theory

$$\boxed{\hat{H} = \sum_{m \neq n} J_{mn} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n}$$



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Spin wave theory

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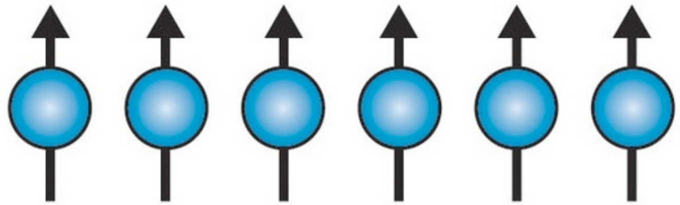


- As a strongly interacting quantum system, for a general spin S, the quantum magnetic Hamiltonian is not easily addressed. However, for large spin S, we can develop a "semi-classical" expansion:
- In problem set I, we developed a representation of the quantum spin algebra, $[\hat{S}_m^+, \hat{S}_n^-] = 2\hbar \hat{S}_m^z \delta_{mn}$, using raising and lowering (ladder) operators – the **Holstein-Primakoff spin representation**,

$$\hat{S}_m^z = \hbar(S - a_m^\dagger a_m)$$

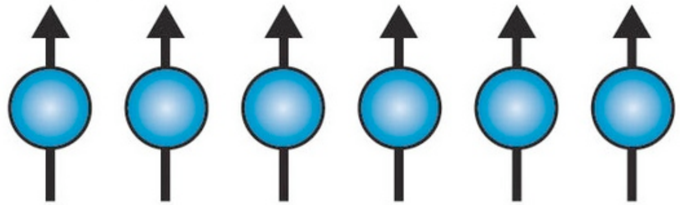
$$\hat{S}_m^- = \hbar\sqrt{2S}\, a_m^\dagger \left(1 - \frac{a_m^\dagger a_m}{2S}\right)^{1/2} \simeq \hbar\sqrt{2S}\, a_m^\dagger + O(S^{-1/2})$$

$$\hat{S}_m^+ = (\hat{S}_m^-)^\dagger \simeq \hbar\sqrt{2S}\, a_m + O(S^{-1/2})$$

where, as usual, $[a_m, a_n^\dagger] = \delta_{mn}$.

Spin wave theory

$$\boxed{\hat{H} = -J\sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}}$$



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Spin wave theory

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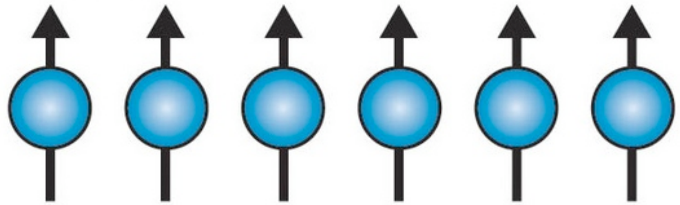

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Spin wave theory

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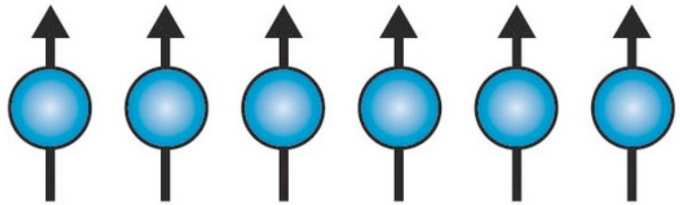

- Defining spin raising and lowering operators, $\hat{S}^{\pm}_m = \hat{S}^x_m \pm i\hat{S}^y_m$,

$$\hat{H} = -J \sum_m \Big\{ \underbrace{\hat{S}^x_m \hat{S}^x_{m+1} + \hat{S}^y_m \hat{S}^y_{m+1}}_{\frac{1}{2}(\hat{S}^+_m \hat{S}^-_{m+1} + \hat{S}^-_m \hat{S}^+_{m+1})} + \hat{S}^z_m \hat{S}^z_{m+1} \Big\}$$

- Using Holstein-Primakoff transformation,

$$\hat{S}^z_m = \hbar(S - a^\dagger_m a_m), \quad \hat{S}^-_m \simeq \hbar\sqrt{2S}\, a^\dagger_m, \quad \hat{S}^+_m \simeq \hbar\sqrt{2S}\, a_m$$

expansion to quadratic order in raising and lowering operators gives,

$$\hat{H} \simeq -JN\hbar^2 S^2 - J\hbar^2 S \sum_m (a_m a^\dagger_{m+1} + a^\dagger_m a_{m+1} - a^\dagger_m a_m - a^\dagger_{m+1} a_{m+1})$$

Spin wave theory

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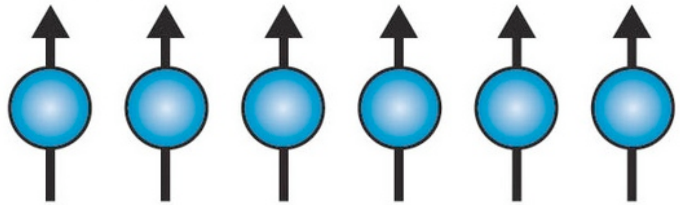

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Spin wave theory

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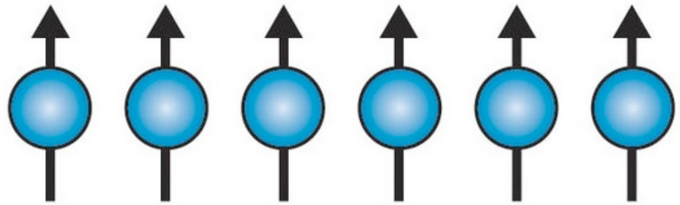

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Spin wave theory

$$\boxed{\hat{H} = -JN\hbar^2 S^2 + J\hbar^2 S \sum_m (a^\dagger_{m+1} - a^\dagger_m)(a_{m+1} - a_m) + O(S^0)}$$

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

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

- As with harmonic chain, Hamiltonian can be diagonalized by Fourier transformation. With periodic boundary conditions, $a^\dagger_{m+N} = a^\dagger_m$,

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

where sum on $k = 2\pi n/N$, runs over integers n and $[a_k, a^\dagger_{k'}] = \delta_{kk'}$,

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Spin wave theory

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Spin wave theory

- As a result, we obtain

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

where $\omega_k = J\hbar S k^2$ 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.