Concept of a Solid: Qualitative Introduction and Overview.

Classification of Solids

- Condensed matter physics is the same area of physics as Solid state physics

→ Condensed matter physics is broader

→ Includes matter in Solid and Condensed phases.

→ Largest branch of physics

→ Covers a large scope of physical phenomena

→ fundemental aspects of physics

→ Applied physics and technology.

→ Experimental Observations of fundemental phenomena in table-top experiments.

- We are going to focus on the Quantum theory of solids.

- A solid (Dictionary definition): "of stable shape, not a liquid or a fluid, having some rigidity."

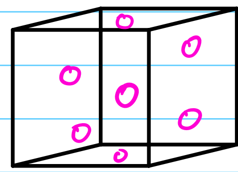
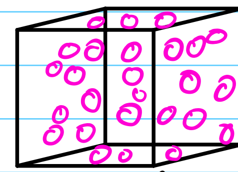
→ Early studies of solids focused on mechanical properties and rigidity of solids (Until 19th century).

→ Example, The Mohs scale of hardness (talc 1, calcite 3, quartz 7, dimond 10). Limited approach to classify solids).

Atomic physics (Solid, collection of ~strongly interacting atoms)

→ It lead to more microscopic concepts of solids

→ from atomic physics point of view

Gas → non-interacting atoms   Liquid → weakly interacting atoms

→ The picture of interacting atoms helped explain the formation of solids by pressure or reduced temperature due to increasing interactions between atoms.

→ Atomic physics and chemical analysis gave a classification of solids according to their chemical composition.

→ Identifying the Atomic Constituents of a solid is important but it provides Limited Insights into basics of condensed matter.

Crystalography : Classification of solids according to their crystaline structure.

→ The discovery of X-ray crystalography expanded the view of the atomic model.

→ The atomic (chemical) view became, strongly interacting atoms arranged in a periodic structure. (This statement is not true for non-crystaline matterials → Amorphous, Glasses, ...).

→ When a new matterial is discovered the first step is characterization → Chemical and Structural Analyses.

Electromagnetic and thermal properties are also used to classify solidis.

→ The resistivity ρ one of the most used quantities (It is a scalar quantity or a symmetric tensor that depends on temperature and can be messured to a great precision.)

→ ρ is a macroscopic quantity but it provides deep insights into the microspics of solids

→ The classification according to ρ (metal, semimetal, semiconductor, insulator).

→ The division between the classes of the ρ classification is approximate but this classification is very useful for studies of solids and applications.

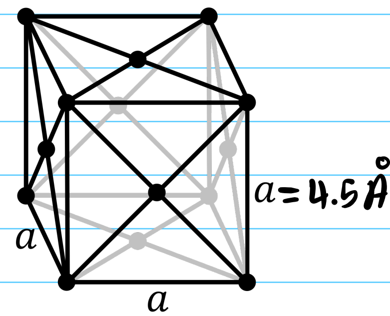
Chemical and Structural Classifications	Electromagnetic and Thermal Classification
— Based on interacting atoms.	— The use of external probes that are used to classify solids.
— Expects the prediction and explanation of solid's properties by the adjustment or perturbation of the constituent atoms.	— Probes collective phenomena
— Does not capture collective or cooperative effects in solids	— Requiers models based on excitations.
— Describes ground state properties	

Two models for solids

A First Model of Solids: Interacting Atoms

Consider the Al metal. Properties according to different classifications

- Mechanical: Soft metal (2–2.9 Mohs scale).
- Crystalography: Face-centered-cubic (FCC) with a lattice constant $a = 4.5\,\mathring{A}$



- Electric conduction: Good conductor at $20^\circ C$ ($\rho = 2.8 \times 10^{-6}\,\Omega cm$).

  Superconductor at $T = 1.19\,K$.

How do we explan the properties of Al and its differences from other metals?

→ Straightforward approach, chemical and atomic description that considers metal Al as a collection of interacting Al atoms.

→ Al atoms have $Z = 13$ (Atomic #). 13e and 13p (for neutral atom).

→ Electron configuration $\underbrace{(1S)^2 (2S)^2 (2P)^6}_{\text{Core electrons}} \underbrace{(3S)^2 (3P)^1}_{\text{Outer valence electrons}}$

→ In the atomic picture we have

  - Cores: nucleus and tightly-bound core electrons.

- Moving arround the cores we have itinerant (nearly-free) electrons
- For Al the core has $Z_{eff} = 3$ and we have nearly 3-free electrons per core.
- The nearly free electrons and the cores effectivly move in a potential set by their mutual interactions.
- We need the Schrödinger equation (Dirac equation in case of relativistic effects)
- The forces: Electromagnetism ✓
  Gravity ✗ } too feeble
  The weak force ✗ }
  The strong force ✗ too short range
- This problem is not easy to solve (10^{23} interacting particles for every cm^3).
- Even if avalable the solution to this problem is most likely to have obscure and non-useful physics
- We need approximate methods.

A second model: Elementary Excitations

A different approach is based on Emergence

In Quantum Mechanics (QM) and Quantum Field Theory (QFT) emergence of excitations is a convinient description when discussing excited states

Examples: 1) An electron in a harmonic potential $\left(\frac{1}{2} m \omega^2 x^2\right)$.

→ Energy Spectrum defined by the quantum # n ($n \in \mathbb{Z}$), where $E_n = (n+\frac{1}{2})\hbar\omega$

→ Ground state energy $E_0 = \frac{1}{2}\hbar\omega$.

→ Quanta of Excitation can be created and destroyed in any non-negative integer multiple of $\hbar\omega$ energy states.

2) The electromagnetic field

→ Collection of quantized particle-like excitations (photons)

→ Photons are characterized by $\vec{k}$ (wavevector), $\hat{\epsilon}$ (polarization), and an energy $\hbar\omega = \hbar c|\vec{k}|$ (c is the speed of light).

Elementary excitations in solids can be (1) Quasiparticle Excitations or (2) Collective Excitations.

Quasiparticle Excitations are usually Fermions that resamble well-defined excited states of non-interacting real particles in the solid

Collective Excitations are usually Bosons that do not resamble their constituent real particles.

→ The most natural language for the elementary excitation model is Second Quantization.

This is since elementary excitations can be created and annihilated. These excitations also need to be symmetric (Bosons) or antisymmetric (Fermions).

These properties can be described by the creation and annihilation operators and their commutation and anticommutation relations.

→ Within this approach we can characterize the properties of a solid by identifyng the elementary excitations of the solid, describe their properties and characteristics, and determine their response to external probes

Elementary Excitations of Solids and Liquids

Quasielectrons (electrons in matter) are low-energy quasiparticle excitations. Behave like non-interacting Fermions. They are characterized by energy and other quantum #s, such as, wavevector and spin orientation.
Their properties reflect the environment they move in. For example an electron interacting with other electrons. The electron free mass (m) can change and become an effective mass m^*. The quasielectron has charge $-|e|$ and spin. The excitation energies of quasielctrons are $\sim$ Coulumb interaction between 2 electrons separated by a lattice constant a ($e^2/a \simeq 5\,eV$), and the velocity of these quasi particles is $v \simeq e^2/(am) \simeq 10^8\,cm/sec$.

Holes are anologous to positrons in relativistic quantum mechanics. They result from the removal of an electron or quisielectron from an occupied state. These quasiparticles are Fermions with charge $|e|$, spin $\frac{1}{2}$, and velocities and masses (most of the time) to quasielectrons. when electrons are injected or removed in a solid due to tunneling or emmission, the electrons are treated as single particles without and the holes are treated separately.

Phonons are collective excitations (Bosons) associated with lattice vaibrations and sound waves. They are characterized by a wavevector $\vec{q}$, a branch or a polarizatin mode index α, and energy $\hbar\omega$. Typical energies of phonons are $K_B T_D$ (K_B is the Boltzman constant and T_D is the Debye temperature). $T_D \sim 300K$ then $\hbar\omega \simeq 25\,meV$.

Plasmons collective excitations associated with the collective motion of the electronic charge density (Plasmons are Bosons). Characterized by a wavector $\vec{q}$ and an energy of the order of the plasma energy

$$\hbar\omega_p = \hbar\,(4\pi n e^2/m)^{1/2} \quad \text{in 3D}$$

n is the density of valence electrons per unit volume. For typical solids $\hbar\omega_p \simeq 10\, eV$. This value is smaller (by an order of magnitude) for low-density electron or hole systems (Semimetals or degenerate Semiconductors).

Magnons are collective excitations (Bosons) that result from spin waves or spin excitations that result from spin reversal in an ordered magnetic system. Typical energies of magnons are $K_B T_C$ (T_C is the Curie or Néel temperature). This energy is in between ~100 meV and ~40 μeV.

Polarons are a special quasielectrons in crystals. Polarons can be seen as an electron or a hole moving through a solid and carrying a lattice deformation or strain with it. The lattice strain can be expressed as excitations of phonons. Then polarons are an electron (or a hole) accompanied with a cloud of phonons. Polaron and polaron effects mean effects arrising from electron-phonon interactions.

Excitons are elctron-hole bound or quasibound state. They are similar to positronium, and they often behave as Bosons that can decompose to their two fermion components or radiatively destroyed. Excitons exist in semiconductors and insulators, and ther binding energies are ~ 25 meV in 3D.

Superconducting Quasiparticles are Fermions that describe the electronic excited state of a superconductor. They are also called Cooper particles or Bogoliubons. These are not cooper pairs (cooper pair condensation into same ground state leads to supper conductivity) instead they are excitations above the ground state. Then, they are linear combinations of quasielectrons an holes. Their typical energies are of the order of the superconducting transition temperature ~ 10^{-5} and 10^{-2} eV.

Rotons are special kind of phonons associated with a local minimum in the dispersion relation at a finite wavevector. Excitation in a Bose-Einstein condensate with a minimum in the excitation spectrum at finite $\vec{K}$. Rotons exist in He^4 (Superfluid) with an energy of 1 meV.

External Probes

To determine the properties of solids, experimental measurments are performed under well defined conditions. Equilibrium conditions, temperature and external static fields are predetermined. Dynamical conditions, dynamical quantities are exchanged with the environment (Energy, momentum, angular momentum, etc.). In the dynamic case the exchange is mediated by quanta that is refered to as test probe particles.

Photons. Electromagnetic probes are the most comon probes for solids. They are used to probe the absorbtion, reflection, photo emission spectra. The range of energies of this probe spans the EM spectra (Radiowaves for metals $\hbar\omega \simeq 10^{-8}$ eV and γ-rays for the Mössbauer effect, $\hbar\omega \simeq 2\times10^{6}$ eV).

Electrons are used in a variety of ways to probe solids. Tunneling junctions, and electrical contacts inject electrons. Electron beams use electrons as scattering particles. The energies of the probing electrons in experiments are ~ 100 meV ~ 2 eV for STM, ~ 1 meV for supperconductive tunneling, ~ 1 eV for semiconductor tunneling and $\sim 10 \sim 100$ eV for low-energy electron difraction of solid surfaces (~ 100 KeV to 1 MeV for high-energy electron microscopy).

Positrons. Electron-positron interactions provide useful information about about the electronic properties of solids via positron annihilation. Photons are emitted when positrons are annihilated. The study of the emmited radiation gives information about the solid's electronic structure

Neutrons. Neutron scattering is the standard probe of magnetic structures, phonons, magnons, and other collective excitations, since neutrons are neutral particles with a magnetic moment.

Muons and Pions. They are not common probes. Muons are more versitile than pions and are used to probe heavy electrons. Their magnetic moments and decay modes can provide unique information about solids

Protons can be used to study crystal structure. This is done by examining their trajetories in the solid.

Atoms. Light attoms are used to probe surfaces, and sometimes to probe deep in the solid. They are also used as scattering particles (similar to electrons).

Dispersion Curves

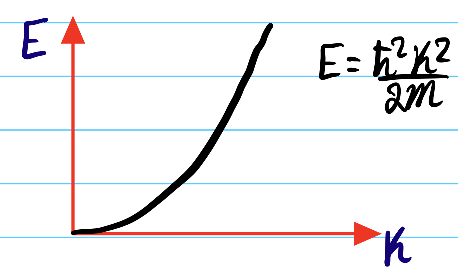
→ All the probing particles are characterized by E (energy) and $\vec{k}$ wave-vector.

→ Probing particles exis in vacuum (free space).

→ Examples:

1) A massive particle of mass m. The dispersion curve is the relation between E and the wavevector k (in free space momentum $P=\hbar k$).

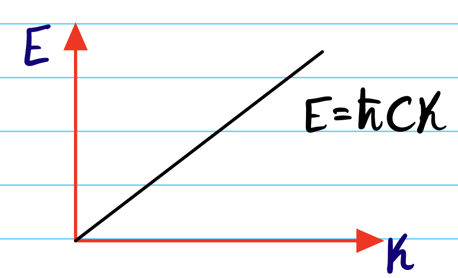
$$E=\frac{p^2}{2m}=\frac{\hbar^2 k^2}{2m} \quad \left(\text{free space} \rightarrow \underset{P=\hbar k}{\text{Translational invarience}}\right)$$



2) A relativistic particle of mass m

$$E=\sqrt{p^2c^2+m^2c^4}=\sqrt{\hbar^2k^2c^2+m^2c^4}$$

if the particle is massles, for example a photon, $E=\hbar c k=\hbar\omega$, where $\omega=ck$.

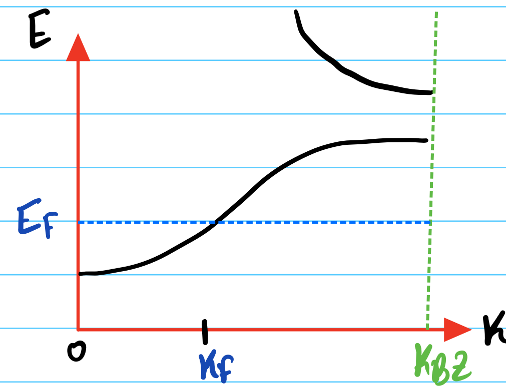


→ In solids or liquids elementary excitations are also defined by E (or frequency ω) and $\vec{k}$.

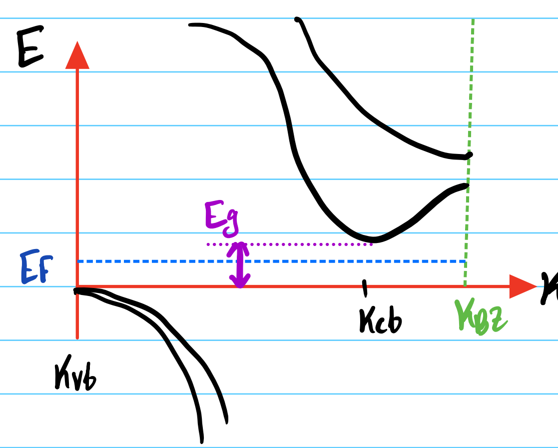
→ The functional dependence of the energy on the wavevector, i.e., the dispersion relation, is one of the most fundemental properties of the excitations and it is essential to determine.

→ The quasielectrons dispersion can be used to classify solids

→ Metals, have no gap in the spectrum and have a Fermi surface

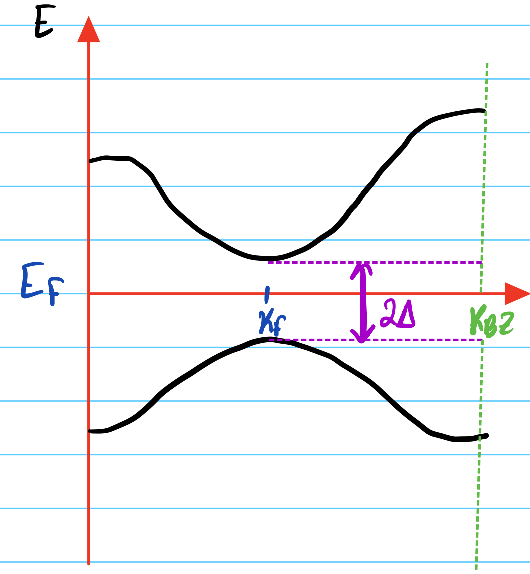


→ Semiconductors and insulators, have electronic gaps of order 0.1 – 10 eV. These gaps are caused by the ion-core potentials and and relate to unique locations in k-space.



→ Superconductors also display a gap. The gap in SC results from dynamic interactions and $2\Delta < 100\,meV$. The gap 2Δ determines the minimum energy requiered to creating both a superconducting quasielectron and a superconducting quasihole.

→ The gap of a superconductor is much smaller than the gap of a semiconductor ($2\Delta = 0.3\,meV$ in aluminum).
→ The gap of superconductors appears at what, in the normal state, was the fermi surface of the metal.
→ The semiconducting gap and the superconductive gaps are very different.



→ It is useful to express the dispersion relation near a minimum or a maximum where the quadratic dispersion is appropriate. for example, assume that $E(\vec{K})$ has a minimum at $\vec{K}_0$, then

$$E(\vec{K}) = \frac{1}{2}\hbar^2 (\vec{K}-\vec{K}_0) \cdot A \cdot (\vec{K}-\vec{K}_0)$$

where $A_{ij} = 1/m^*_{ij}$ and m_{ij} is the effective mass tensor.

For an electron in freespace $A_{ij} = m^{-1}\delta_{ij}$.

In solids, the effective mass (m^*) may differ substantialy from the free electron mass.

→ In InSb $m^* \simeq 0.01m$ near the conduction band minimum. This is caused by the crystal potential that leads to the existance of a gap.

→ In Na metal the Fermi surface is a sphere (very good approximation) of radius k_F, hence

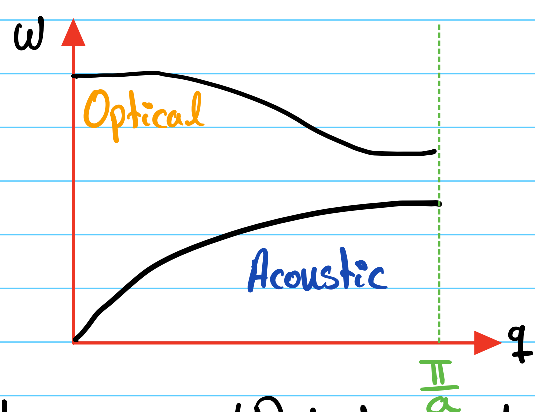
$$E(\vec{k}) = \frac{\hbar^2}{2m^*} |\vec{k} - \vec{k}_F|^2 \quad \text{(for electrons and holes)}$$

Here $m^* \cong 1.25\, m$. The enhancement of 25% over the electron mass is due electron-phonon and electron-electron interactions.

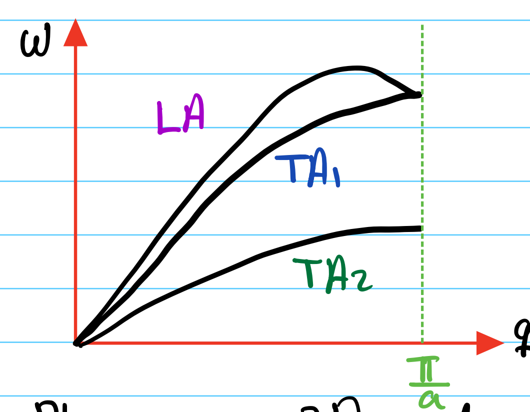
→ Dispersion relations of collective excitations

→ In restricted regions of the spectra, analytical approximations are usually made. For example for acoustic phonons near $|q|=0$

$$\hbar \omega_\alpha = \hbar v_\alpha |q| \quad (\text{for acoustic mode } \alpha).$$



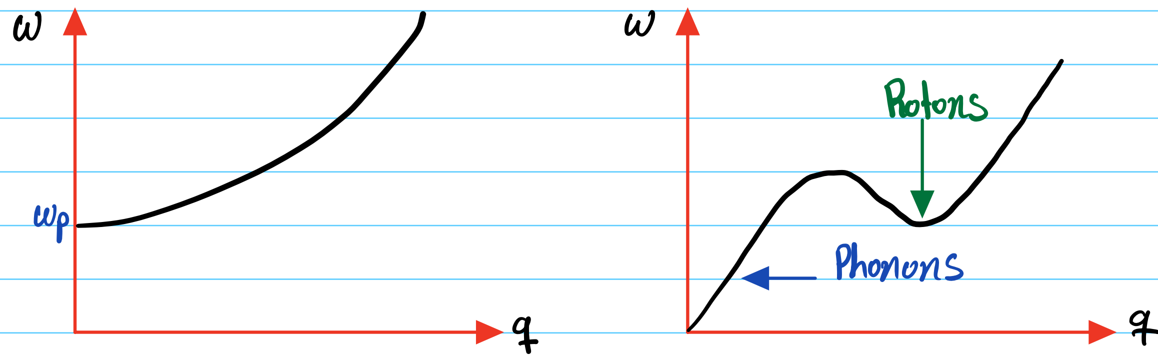
Phonons in a 1D diatomic chain with lattice constant a.



Phonons in a 3D solid with one atom/cell.

where v_α is the speed of propagation of mode α.

→ Other dispersions of collective excitations



→ The determination an interpration of elementary quasiparticles dispersion can be complicated. However, there is a scheme (investigational approach) that can be outlined.

1) Define the bare elementary excitations by means of a Hamiltonian formalism.

2) Solve the equations of motion to determine the dispersion curves for the quasiparticle excitations

3) Solving for the final spectrum of the excitantions including the nessesary interactions among the quasiparticles.

4) Include the effects of external probes and their interactions with the excitations

5) Solving the new coupled equations to determine the response functions of the condensed matter system.

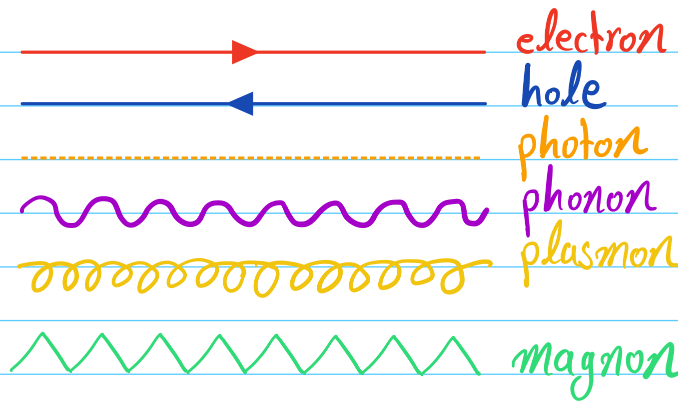
(1)–(2) Are handled by ordinary quantum mechnics, using the Schrödinger equation for a one-body in an external potential.

(3)–(5) Are many body aspects that can be evaluated using 2^{nd} quantization and Green's functions techniques. It is convenient to express the physical processes in these steps graphically via Feynman diagrams.

Graphical Representation of Elementary Excitations

Elementary excitations, probes, and their interactions can be graphically represented in Feynman diagrams.

- Time develops from left to right or bottom to top.
- Elementary excitations are depicted by lines of different kinds for different excitations.
- The lines are labeled by the excitations quantum #s.

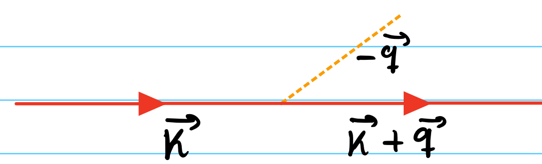


Interactions Among Particles

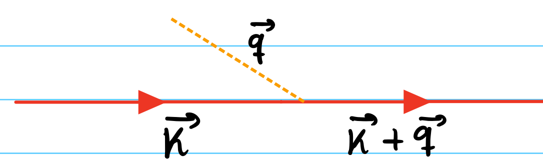
The last 3 parts in the condensed matter system analysis requier the description of interactions between elementary excitations and with the probe particles.

Quasiparticles - Boson Interactions

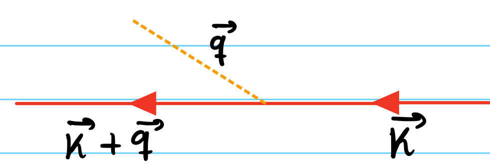
An electron with momentum $\vec{k}$
emits a photon with momentum $-\vec{q}$
and scatters into a state with momentum $\vec{k}+\vec{q}$



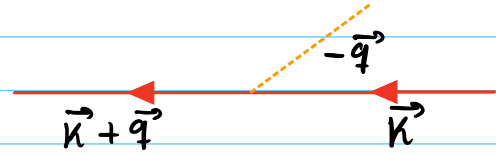
An electron with momentum $\vec{k}$
absorbs a photon with momentum $\vec{q}$
and scatters into a state with momentum $\vec{k}+\vec{q}$



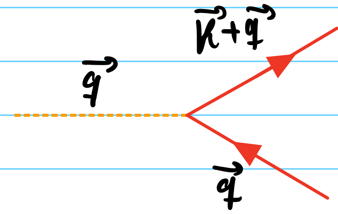
A hole with a wavevector $-\vec{k}-\vec{q}$
absorbs a photon with momentum $\vec{q}$
and it scatters to a state with momentum $-\vec{k}$



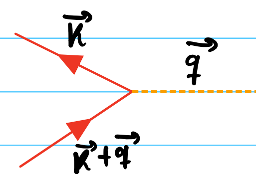
A hole with a momentum $-\vec{k}-\vec{q}$
emits a photon with momentum $-\vec{q}$
and it scatters to a state with momentum $\vec{k}$



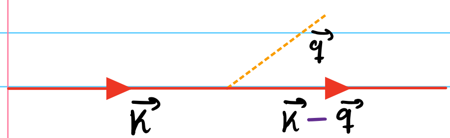
A photon with a wave vector $\vec{q}$ creates
an electron with momentum $\vec{k}+\vec{q}$ and a
hole with momentum $-\vec{k}$

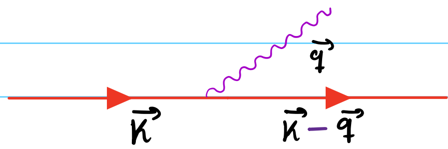


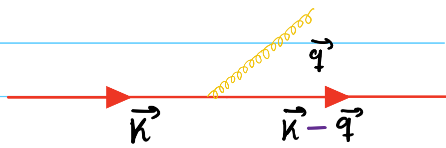
The annihilation of an eletron with a momentum
$\vec{k}+\vec{q}$ and a hole with wavevector $-\vec{k}$ to create
a photon with a wavevector $\vec{q}$.



Interactions with other bosons







Electron-photon interaction: Optical absorbtion and emission
Photoemission
X-ray scattering
Compton Scattering
Raman Scattering
Cyclotron Resonance

Electron-phonon interaction: Electric and thermal resistance
Ultrasonic attenuation
Polaron formation
Superconductivity

Electron-plasmon interaction: Electron energy loss of fast electrons through a solid

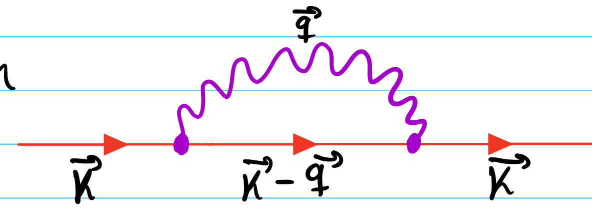
Electron-magnon interaction: Magnetic resonance
Transpor in magnetic materials.

Quasiparticle-Quasiparticle Interactions

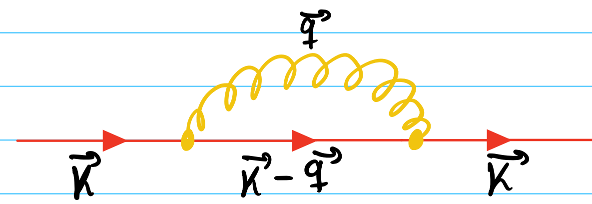
Quasiparticles can interact with eachother via residual interactions or indirectly via the exchange of a collective excitation

Electrons and Hole Self-energy.

The emission and reabsorbtion of a boson "dresses" the "bare" quasiparticle. This process produces changes in the energy and effective mass of the quasiparticle. For electrons this could lead to the formation of a polaron or a plasmonic polaron.



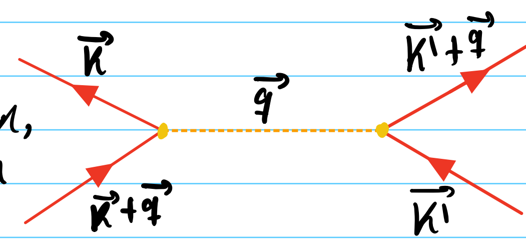
(a)



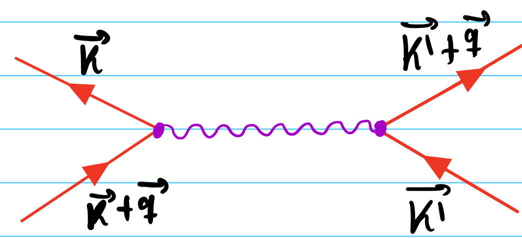
(b)

Electron-electron and Hole-hole Interaction

This leads to quasiparticle-quasiparticle scattering via the residual Coulomb interaction, which can be vived as the exchange of a photon or in some cases a phonon, magnon, or a plasmon. The phonon exchange can lead to an effective attraction between quasielectrons and to a superconducting transition.



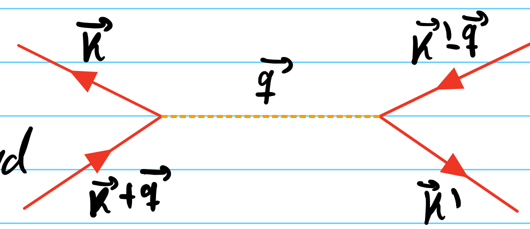
(a)



(b)

Electron-hole Interaction

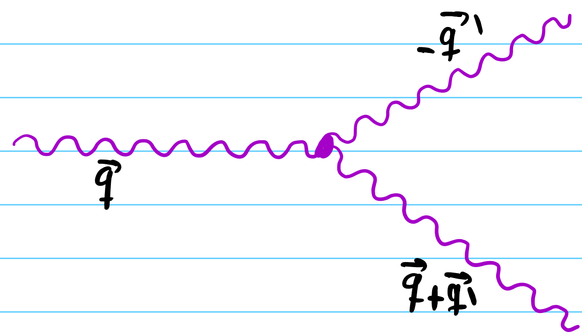
Electrons and holes interact via Coulomb by exchanging a photon (plasmons, magnons, and phonons). Thes processes lead to screening the formation of excitons and other many body effects.



Collective Excitations Interactions

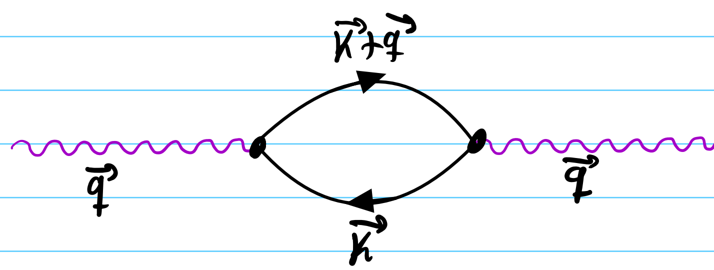
Collective excitation can be seen as quanta of harmonic oscillators via 2^{nd} Quantization.

Any anharmonicity leads to the dressing as well as the decay of the mode into a multiplicity of other modes



Ferroelectricity and Thermal expansion

Collective excitation can be also "dressed" by the creation of a virtual quasielectron-hole pair



Mode softening phase transitions