PHY 555

Solid State Physics or Condensed Matter Physics

Course Grading

There will be one midterm and a final exam. Midterm will be a short (1.5 h long) exam. The final exam will cover everything. Exams will be very much in line with homeworks. Each exam will be only 25% of the course. Homework will be another 50% of the course.
At the end of the semester there will also be a journal club style presentation on a paper chosen by you, from a list of papers I will make available. This will be graded as a homework.

Assignments : 50% Every second week (7 assignments, Brightspace)
Midterm I : 25% Date Oct 15
Final: 25% .

What is a solid?

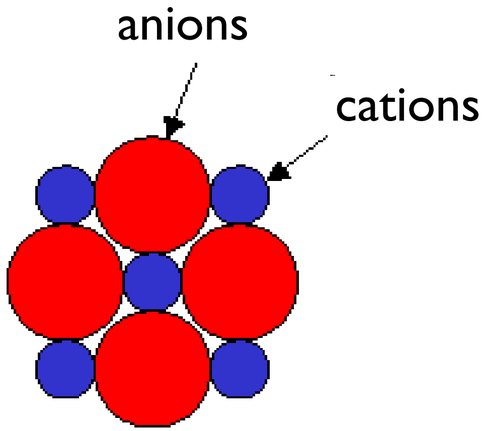
Result of interactions between ~10^{23} atoms yield a geometric structure that maintains its shape.

How can we understand the properties of a solid in terms of its atomic composition and geometric structure?

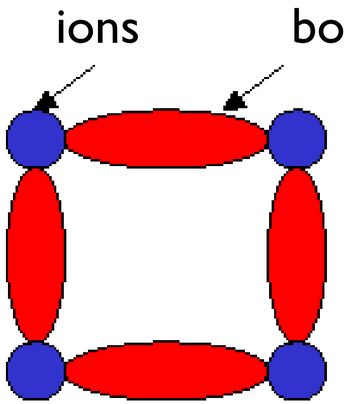
Structure + Composition 

- Structural properties (mechanical properties, crystal structure,surfaces...)
- Electrical properties (resistivity, conductivity, I/V characteristics, Hall effect)
- Thermal properties (specific heat, thermal conductivity)
- Optical properties (color, response to EM fields)

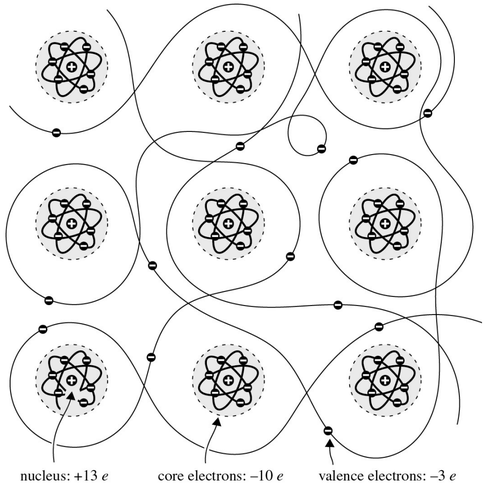
Bonding properties of solids: How much of the individual atom is kept?



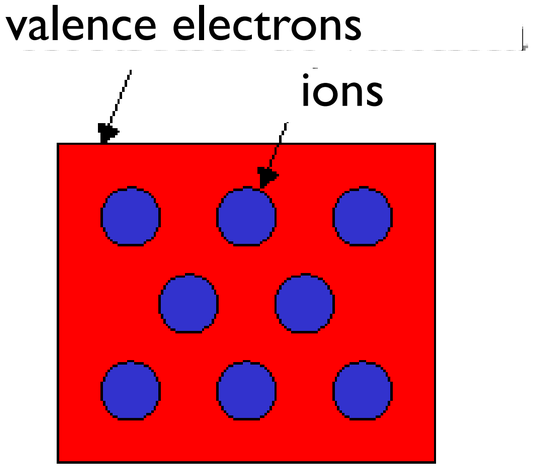
Ionic



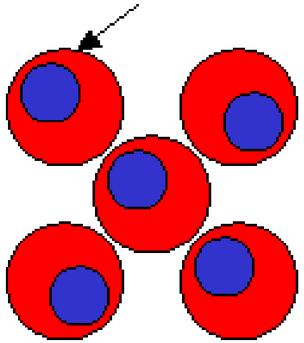
Covalent



MarvinCohen_Fig.1.1



Metallic



Molecular

Just considering electrical properties there is a huge variation

Solid	Resistivity
Insulator	10^{14}-10^{22} Ωcm
Semiconductor	10^{-2}-10^{8} Ωcm
Metal	10^{-6} Ωcm
Superconductor	0

} 28 orders of magnitude!!

Well, we can use a theory of everything, we know the equation for it!

“The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

Dirac, 1929

$$H = \sum_{\alpha} \frac{p_\alpha^2}{2M_\alpha} + \sum_{i} \frac{p_i^2}{2m} + 1/2 \sum_{\alpha \neq \beta} \frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|} + 1/2 \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} - \sum_{i\alpha} \frac{Z_\alpha e^2}{|R_\alpha - r_i|}$$

- Suppose each electron's wavefunction is represented on a cubic grid with m=50 points per spatial axis. The many-electron wavefunction lives in 3N dimensions, requiring m^(3N) amplitudes.

•Evaluating the energy requires: $E = \langle \Psi | H | \Psi \rangle$

•Brute-force scaling: $O(N^2\, m^{(3N)})$ operations
N electrons → wavefunction has m^(3N) amplitudes
Electron-electron terms add ~N^2 factor
Variational minimization: need ~10^3–10^4 evaluations

Assumptions:
• cubic grid with m=50 points/axis;
• Ψ stored as 16 bytes/complex value;

• El Capitan FP64R max ≈1.742e18 (exa)FLOPS;

• RAM ≈ 5.44 PB.

Time to converge (best-case at El Capitan)

N	Ops per energy eval	Time for 10^3 evals	Time for 10^4 evals
3	1.758E+16	1.009e+01 s (**10.1 s**)	1.009e+02 s (**100.9 s**)
4	3.906E+21	2.242e+06 s (**26.0 d**)	2.242e+07 s (**259.5 d**)
5	7.629E+26	4.380e+11 s (**1.39e+04 yr**)	4.380e+12 s (**1.39e+05 yr**)

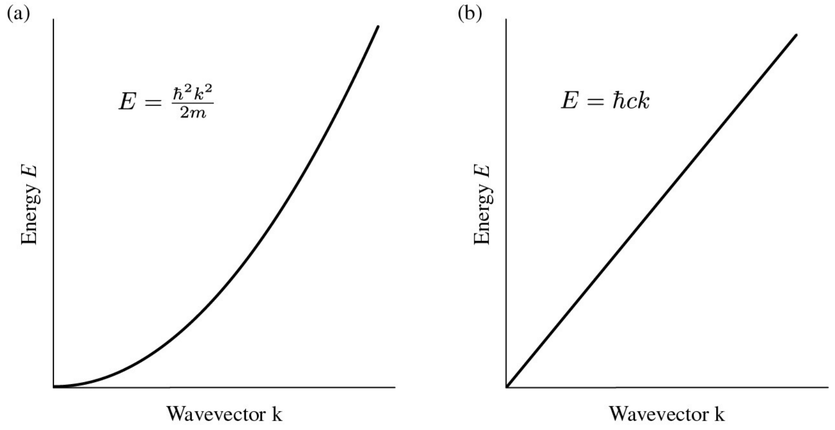
Storage to represent Ψ on the grid (m = 50)

N	m^(3N)	Storage (approx)
3	1.953E+15	3.12e+01 PB
4	2.441E+20	3.91e+00 ZB
5	3.052E+25	4.88e+05 ZB

Elementary excitation model

Description of solids in the elementary excitation model:
Excitations can emerge when the system is not in the ground state. We need to know the energy spectrum and the density of states (i.e statistics of the system, fermions or bosons)

Interaction among different excitations: How they appear, disappear and interact with external probes
Quasiparticles (usually fermions) not too different from the excited states of the particles they arise from
Collective excitations (usually bosons): very different from the underlying particles excitations.
Generalized harmonic oscillators (2nd Quantization)



MarvinCohen_Fig.1.2

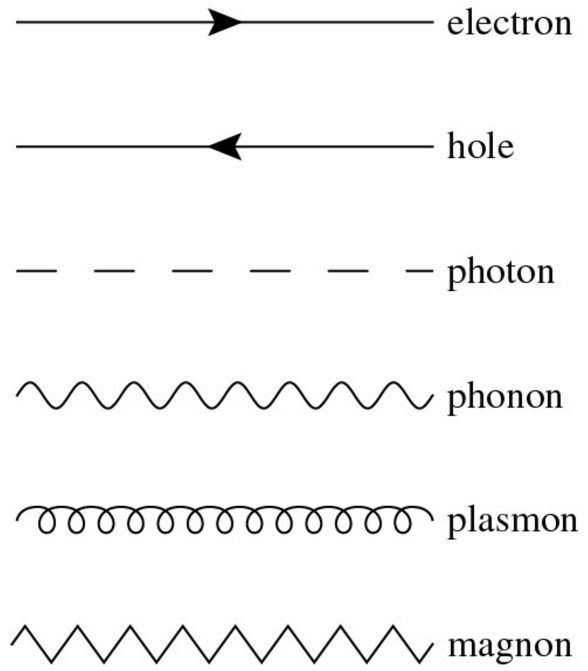
Quasiparticles

- **Quasielectrons**: or electrons. Particles that behave like non-interacting electrons in low lying excited states. = electron-like, long-lived excitations near the Fermi surface with renormalized parameters (m→m*). Their characteristic scales in ordinary solids are a few eV (coulomb energy in energy and 10^8 cm/s in velocity.

$$E_C \sim \frac{e^2}{4\pi\varepsilon_0\, a} \approx \frac{14.4\ \text{eV}\cdot\text{Å}}{a(\text{Å})} \approx 4.8\ \text{eV} \quad (a = 3\ \text{Å}).$$

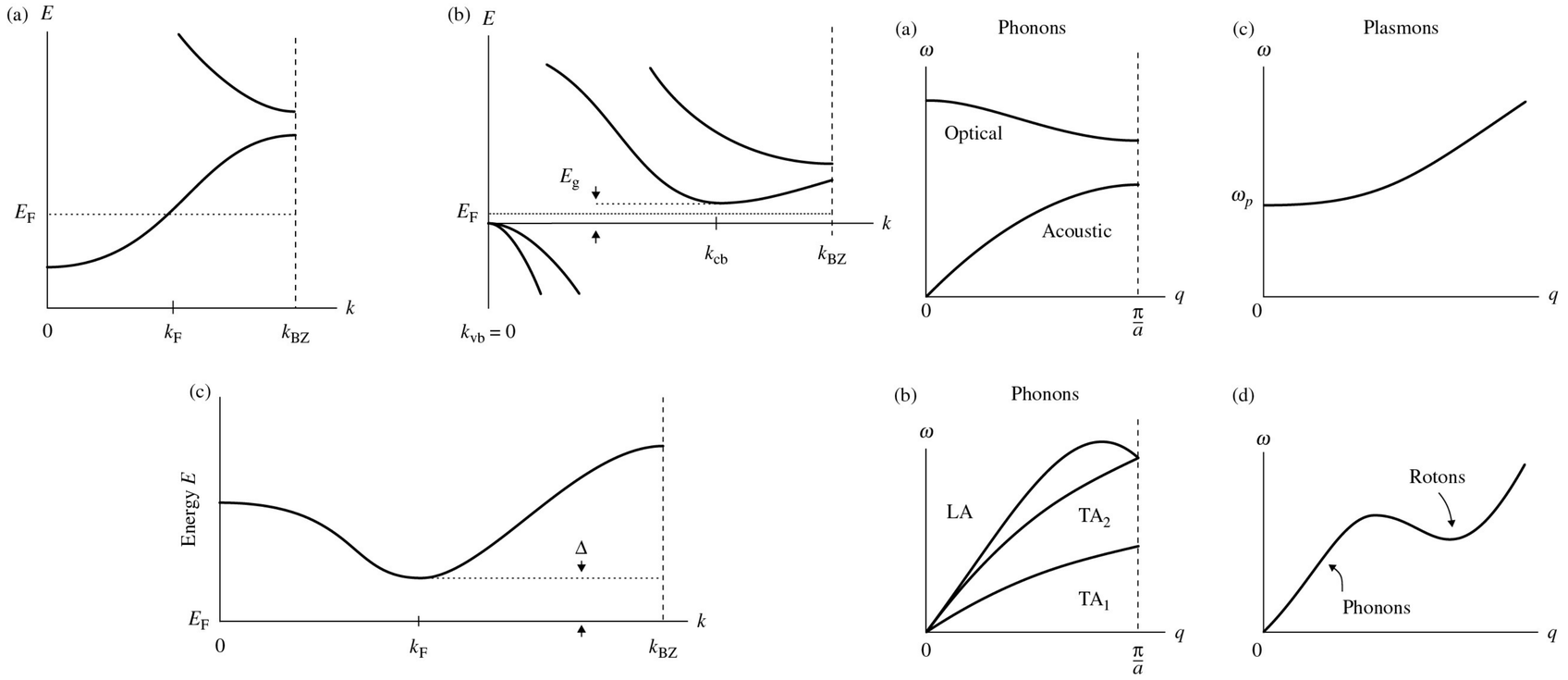
$$\tfrac{1}{2}mv^2 \sim \frac{e^2}{4\pi\varepsilon_0\, a} \Rightarrow v \sim \sqrt{\frac{2\,e^2}{4\pi\varepsilon_0\, a\, m}} \approx 10^6\ \text{m/s} = 10^8\ \text{cm/s},$$

- **Hole**: opposite charge of a quasilectron
- **Phonon**: Collective excitation of the lattice (boson). wave vector q, polarization mode and energy hω. Energies of order of K_bT_D (Td room T, 300K, so energies of order of meV)
- **Plasmon**: Collective excitation (boson) of the electrons (charge density fluctuation) Wave vector q and energy of order of classical plasma energy: $h\omega_p \sim 10$ eV for metals but can be much smaller if electron density n is small ($h\omega_p = h(4\pi\, ne\text{^}2 / m)\text{^}(1/2)$)
- **Magnon**: Collective excitation of spins (spin waves). Energies of ~0.0001 eV, but can be as high as 0.1 eV)
- **Polaron**: Type of quasilectron Electron+lattice deformation. Very heavy electron. Can be though as a phonon dressed electron. Binding energies ~ 10-100 meV
- **Exciton**: Bound state of a quasilectron and a hole. Binding energies of 0.025 eV. Typical in semiconductors and insulators.
- **Superconducting quasiparticle**: Fermions, electronic excited states of a superconductor (cooper particles or Bogoliubons). Linear combination of electrons and holes. Energies ~ Tc ~ 10^{-5}-10^{-2} eV

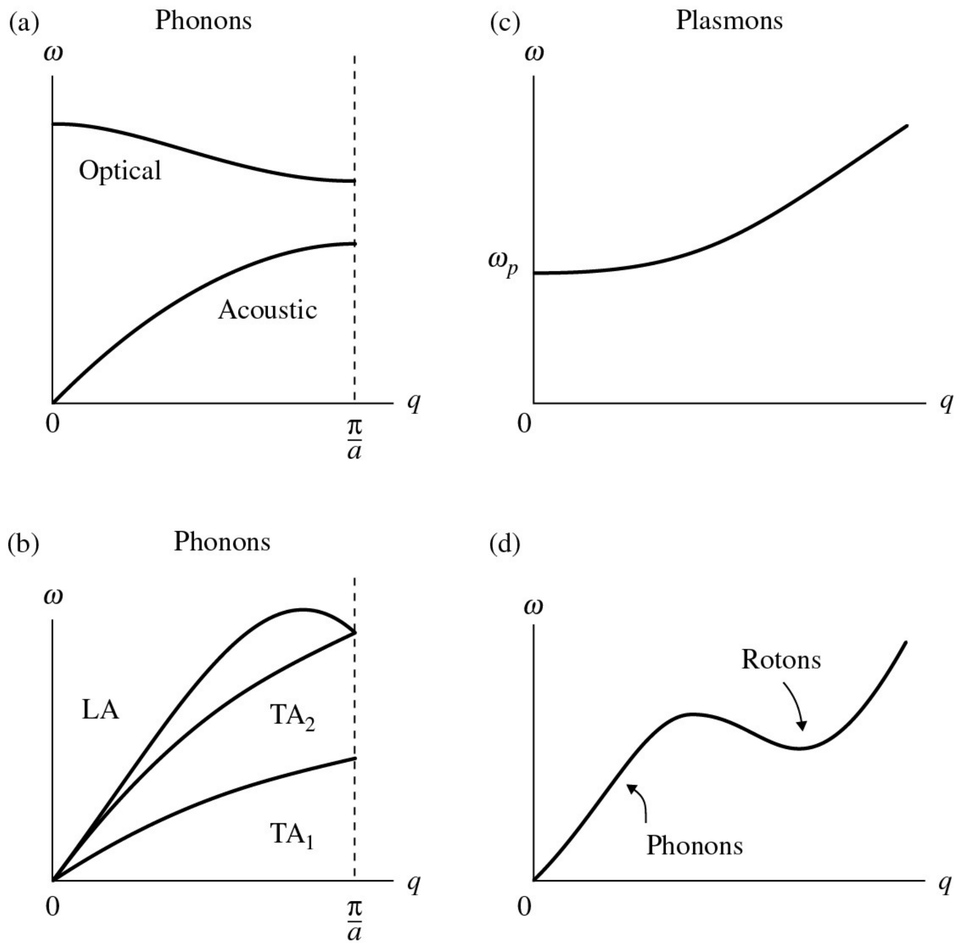


MarvinCohen_Fig.1.5

Dispersion curves

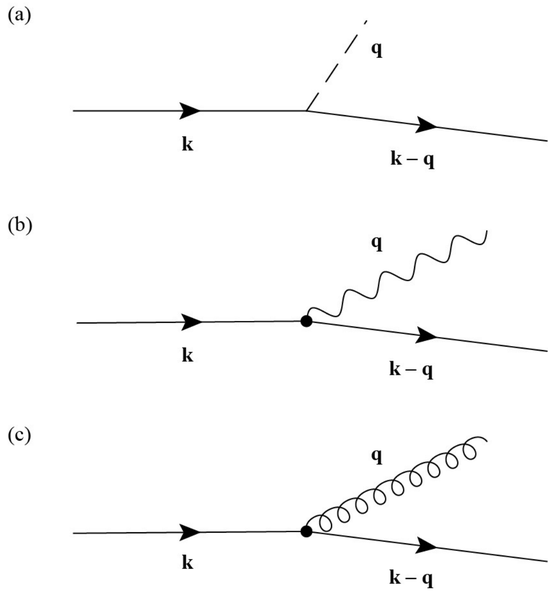


MarvinCohen_Fig.1.3



MarvinCohen_Fig.1.4

Interactions among quasiparticles: quasiparticle-boson



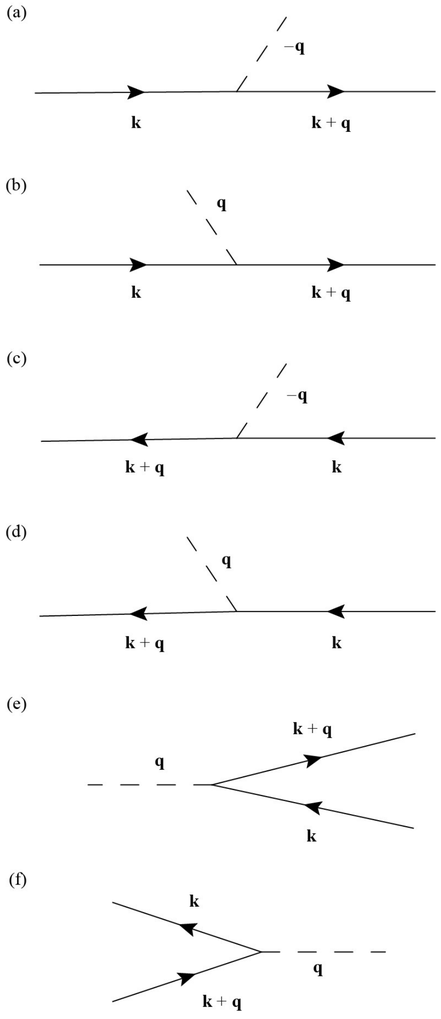
Electron-photon

Electron-phonon

Electron-plasmon

MarvinCohen_Fig.1.7

Interactions among quasiparticles: quasiparticle-boson



Electron (k) emits a photon (-q) scattering into k+q

Electron (k) absorbs a photon (q) scattering into k+q

Hole (-k-q) emits a photon (-q) scattering into -k

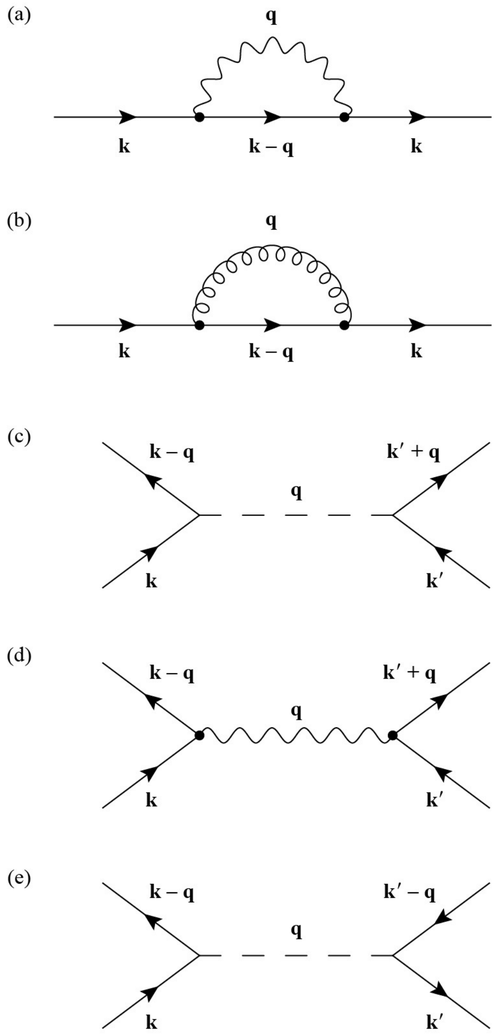
Hole (-k-q) absorbs a photon (q) scattering into -k

photon (q) creates an electron k+q and hole -k

electron (k+q) and hole (-k) recombine or annihilate into photon (q)

MarvinCohen_Fig.1.6

Interactions among quasiparticles: quasiparticle-quasiparticle interactions



Electron self energy (k) emits and absorbs a phonon (q)

Electron self energy (k) emits and absorbs a plasmon (q)

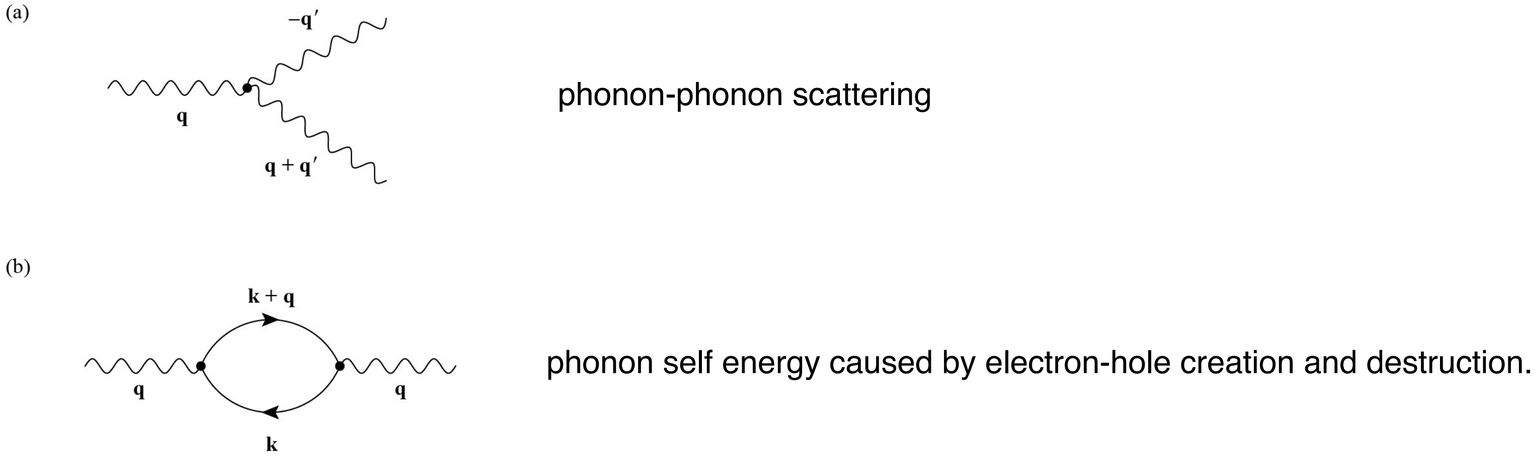
Electron-electron Coulomb interaction or photon exchange

Electron-electron interaction via phonon exchange

Electron-hole Coulomb interaction

MarvinCohen_Fig.1.8

Interactions among quasiparticles: collective excitation interactions

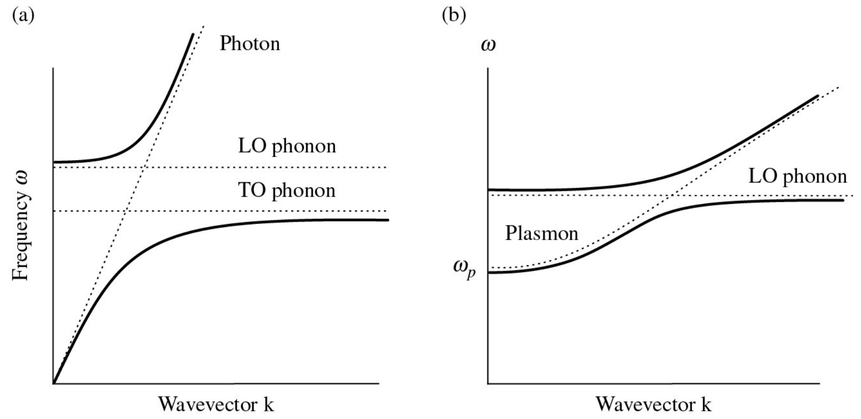


phonon-phonon scattering

phonon self energy caused by electron-hole creation and destruction.

MarvinCohen_Fig.1.9

Interactions among quasiparticles: collective excitation interactions



Couple modes from bare collective excitations
(a) optical phonon-photon complex (polariton) (b) longitudinal optical phonon-plasmon complex

MarvinCohen_Fig.1.10

There are many approximations that we can use to simplify the Sc. eq. for the solid:

- Adiabatic approximation (Born-Oppenheimer) M>>m (Ziman, P. 200)

Separate the ionic problem for the electronic problem

$$H = \sum_\alpha \frac{p_\alpha^2}{2M_\alpha} + \sum_i \frac{p_i^2}{2m} + 1/2 \sum_{\alpha\neq\beta} \frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|} + 1/2 \sum_{i\neq j} \frac{e^2}{|r_i - r_j|} - \sum_{i\alpha} \frac{Z_\alpha e^2}{|R_\alpha - r_i|}$$

$$H = H_e + H_{ion}$$

$$H_{ion} = \sum_\alpha \frac{p_\alpha^2}{2M_\alpha} + \frac{1}{2} \sum_{\alpha\neq\beta} \frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|}$$

$$H_e = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i\neq j} \frac{e^2}{|r_i - r_j|} - \sum_{\alpha i} \frac{Z_\alpha e^2}{|r_i - R_\alpha|}$$

1/M is our small parameter; Kin energy of nuclei is a perturbation in our hamiltonian, the wave function of the coupled system are linear combinations of electronic states that depend parametrically on R. These are the so called adiabatic states.

$$\Psi = \phi_e(R, r)\chi(R)$$

$$H_e\Psi = \chi(R)E_e(R)\phi(R, r)$$

$$H_{ion}\Psi = -\frac{\hbar^2}{2M}\frac{\partial}{\partial R^2}(\phi(R, r)\chi(R)) + V_{ion}(R)(\phi(R, r)\chi(R))$$

$$H\Psi = \phi(r,R)\{-\sum_\alpha \frac{\hbar^2\partial^2}{2M\partial R_\alpha^2} + E_e(R) + V_ion(R)\}\chi(R) - \sum_\alpha \frac{\hbar^2}{2M}(2\frac{\partial\chi}{\partial R_\alpha}\frac{\partial\phi}{\partial R_\alpha} + \chi(R)\frac{\partial^2\phi}{\partial R^2})$$

$$H\Psi = \epsilon\Psi$$

$$H_{ion}^{new}\chi(R) = \epsilon\chi(R)$$

Where H_{ion}^{new} is an eq. for a wave function of the ions alone. This is the basic equation for the calculation of phonons in the adiabatic approximation.

M~10^4 m, so the approximation is very good. But we are ignoring electronic transitions induced by the ionic motion (e-phonon interactions, which give rise to non diagonal terms in the Total Hamiltonian!)

The reduction of the Full wave function to an expression of the type:

$$\Psi(R,r) = \chi(R)\phi(R;r)$$

is not completely correct, because, even if the system was initially prepared in a pure state like the above one, the off diagonal terms will mix (excite) the different electronic eigenstates along the temporal evolution.

Wave function decoupled, Classical nuclei

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m_e}\nabla_i^2 + \sum_\alpha -\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{\vec{r_i}-\vec{r_j}} - \sum_{i,\alpha}\frac{Z_\alpha e^2}{|\vec{r_i}-\vec{R_\alpha}|} + \frac{1}{2}\sum_{\alpha\neq\beta}\frac{Z_\alpha Z_\beta e^2}{\vec{R_\alpha}-\vec{R_\beta}}$$

Fixed potential "external" to e-

Electrons

$$\hat{H}^{el}_{\{\vec{R}_\alpha\}} = \sum_i -\frac{\hbar^2}{2m_e}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r_i}-\vec{r_j}|} + V^{ext}_{\{\vec{R}_\alpha\}}\left(\{\vec{r}_i\}\right)$$

$$\hat{H}^{el}_{\{\vec{R}_\alpha\}}\Psi^{el}_{n,\{\vec{R}_\alpha\}}\left(\{\vec{r}_i\}\right) = E^{el}_n\Psi^{el}_{n,\{\vec{R}_\alpha\}}\left(\{\vec{r}_i\}\right)$$

Nuclei

$$\hat{H} = \sum_\alpha -\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 + E^{el}_n\left(\{\vec{R}_\alpha\}\right)$$

Classical dynamics

$$\vec{F}_\alpha = -\frac{\partial E^{el}_0\left(\{\vec{R}_\mu\}\right)}{\partial\vec{R}_\alpha}$$