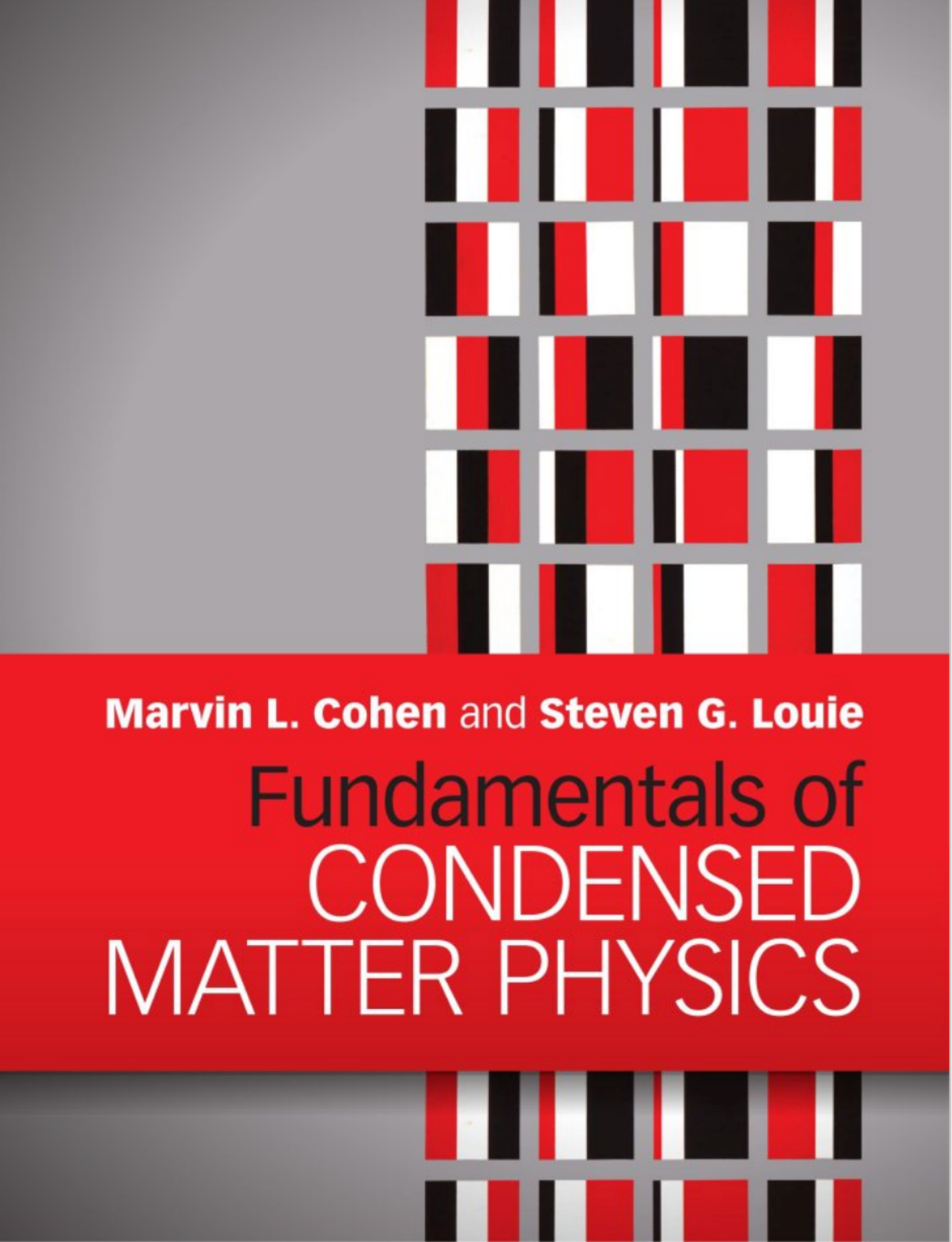


PHY 555

Solid State Physics or Condensed Matter Physics



Marvin L. Cohen and **Steven G. Louie**
**Fundamentals of
CONDENSED
MATTER PHYSICS**

Contents

<i>Preface</i>	<i>page xi</i>
Part I Basic concepts: electrons and phonons	
1 Concept of a solid: qualitative introduction and overview	3
1.1 Classification of solids	3
1.2 A first model of a solid: interacting atoms	4
1.3 A second model: elementary excitations	6
1.4 Elementary excitations associated with solids and liquids	7
1.5 External probes	8
1.6 Dispersion curves	9
1.7 Graphical representation of elementary excitations and probe particles	13
1.8 Interactions among particles	13
2 Electrons in crystals	20
2.1 General Hamiltonian	20
2.2 The Born–Oppenheimer adiabatic approximation	21
2.3 The Hartree mean-field approximation	22
2.4 The periodic potential approximation	22
2.5 Translational symmetry, periodicity, and lattices	23
3 Electronic energy bands	31
3.1 Free electron model	31
3.2 Symmetries and energy bands	33
3.3 Nearly-free electron model	39
3.4 Tight-binding model	43
3.5 Electron (or hole) velocity in a band and the f -sum rule	48
3.6 Periodic boundary conditions and summing over band states	52
3.7 Energy bands for materials	55
4 Lattice vibrations and phonons	63
4.1 Lattice vibrations	63
4.2 Second quantization and phonons	70
4.3 Response functions: heat capacity	77

4.4	Density of states	78
4.5	Critical points and van Hove singularities	83
Part I Problems		89
Part II Electron Interactions, Dynamics, and Responses		
5	Electron dynamics in crystals	101
5.1	Effective Hamiltonian and Wannier functions	101
5.2	Electron dynamics in the effective Hamiltonian approach	103
5.3	Shallow impurity states in semiconductors	107
5.4	Motion in external fields	108
5.5	Effective mass tensor	113
5.6	Equations of motion, Berry phase, and Berry curvature	114
6	Many-electron interactions: the interacting electron gas and beyond	119
6.1	The interacting electron gas or jellium model	121
6.2	Hartree–Fock treatment of the interacting electron gas	123
6.3	Ground-state energy: Hartree–Fock and beyond	126
6.4	Electron density and pair-correlation functions	130
6.5	$g(\mathbf{r}, \mathbf{r}')$ of the interacting electron gas	132
6.6	The exchange-correlation hole	135
6.7	The exchange-correlation energy	136
7	Density functional theory	140
7.1	The ground state and density functional formalism	141
7.2	The Kohn–Sham equations	143
7.3	<i>Ab initio</i> pseudopotentials and density functional theory	149
7.4	Some applications of DFT to electronic, structural, vibrational, and related ground-state properties	151
8	The dielectric function for solids	158
8.1	Linear response theory	158
8.2	Self-consistent field framework	162
8.3	The RPA dielectric function within DFT	163
8.4	The electron gas	165
8.5	Some simple applications	168
8.6	Some other properties of the dielectric function	172
Part II Problems		177

Part III Optical and transport phenomena		
9	Electronic transitions and optical properties of solids	185
9.1	Response functions	185
9.2	The Drude model for metals	189
9.3	The transverse dielectric function	192
9.4	Interband optical transitions in semiconductors and insulators	196
9.5	Electron–hole interaction and exciton effects	201
10	Electron–phonon interactions	218
10.1	The rigid-ion model	218
10.2	Electron–phonon matrix elements for metals, insulators, and semiconductors	222
10.3	Polarons	227
11	Dynamics of crystal electrons in a magnetic field	232
11.1	Free electrons in a uniform magnetic field and Landau levels	232
11.2	Crystal electrons in a static \mathbf{B} -field	234
11.3	Effective mass and real-space orbits	236
11.4	Quantum oscillations: periodicity in $1/B$ and the de Haas–van Alphen effect in metals	238
12	Fundamentals of transport phenomena in solids	245
12.1	Elementary treatment of magnetoresistance and the Hall effect	245
12.2	The integer quantum Hall effect	253
12.3	The Boltzmann equation formalism and transport in real materials	260
12.4	Electrical and thermal transport with the linearized Boltzmann equation	267
Part III Problems		274
Part IV Superconductivity, magnetism, and lower-dimensional systems		
13	Using many-body techniques	283
13.1	General formalism	283
13.2	Interacting Green’s functions	287
13.3	Feynman diagrams and many-body perturbation theory techniques	294
14	Superconductivity	301
14.1	Brief discussion of the experimental background	301
14.2	Theories of superconductivity	306
14.3	Superconducting quasiparticle tunneling	344
14.4	Spectroscopies of superconductors	350
14.5	More general solutions of the BCS gap equation	353
14.6	Field theoretical methods and BCS theory	361

15 Magnetism	365
15.1 Background	365
15.2 Diamagnetism	365
15.3 Paramagnetism	367
15.4 Ferromagnetism and antiferromagnetism	370
15.5 Magnetism in metals	379
15.6 Magnetic impurities and local correlation effects	382
16 Reduced dimensional systems and nanostructures	386
16.1 Density of states and optical properties	386
16.2 Ballistic transport and quantization of conductance	392
16.3 The Landauer formula	397
16.4 Weak coupling and the Coulomb blockade	399
16.5 Graphene, carbon nanotubes, and graphene nanostructures	402
16.6 Other quasi-2D materials	414
Part IV Problems	416
<i>References</i>	427
<i>Index</i>	433

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 TBD

Final: 25% (can replace grade of MT1 or MT2 whichever is lower).

What is a solid?

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

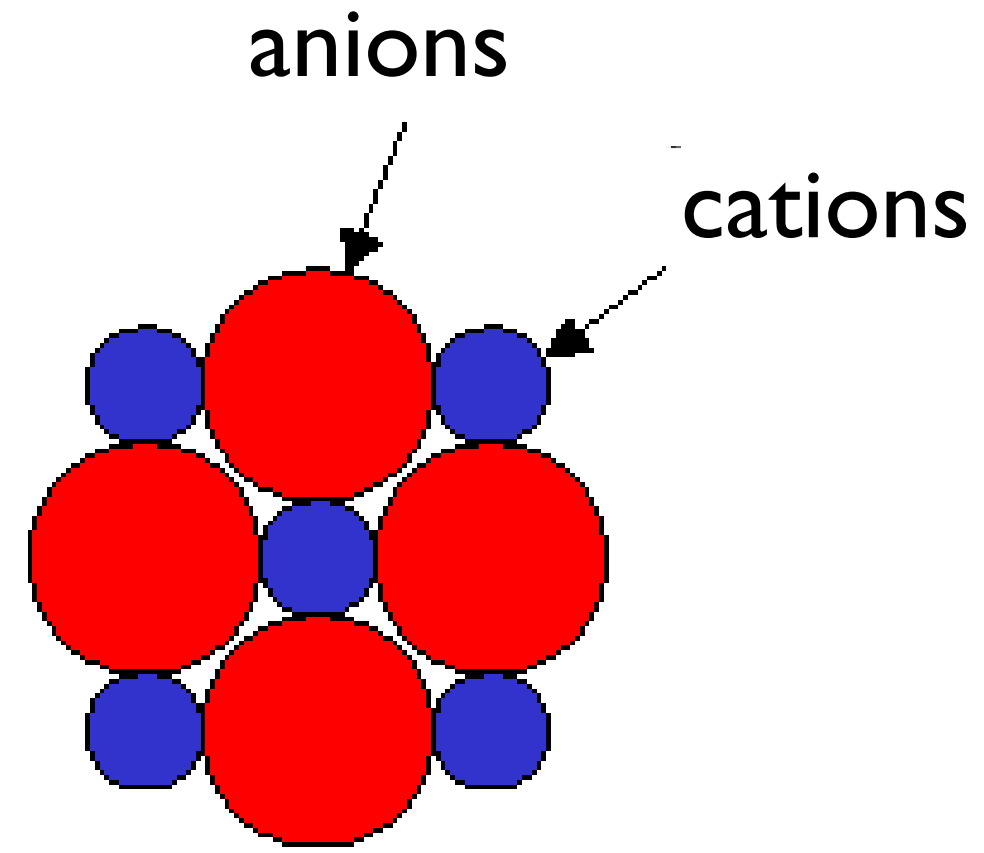
How can we understand the properties of a solid in terms of its atomic composition and geometric structure?

Structure +
Composition

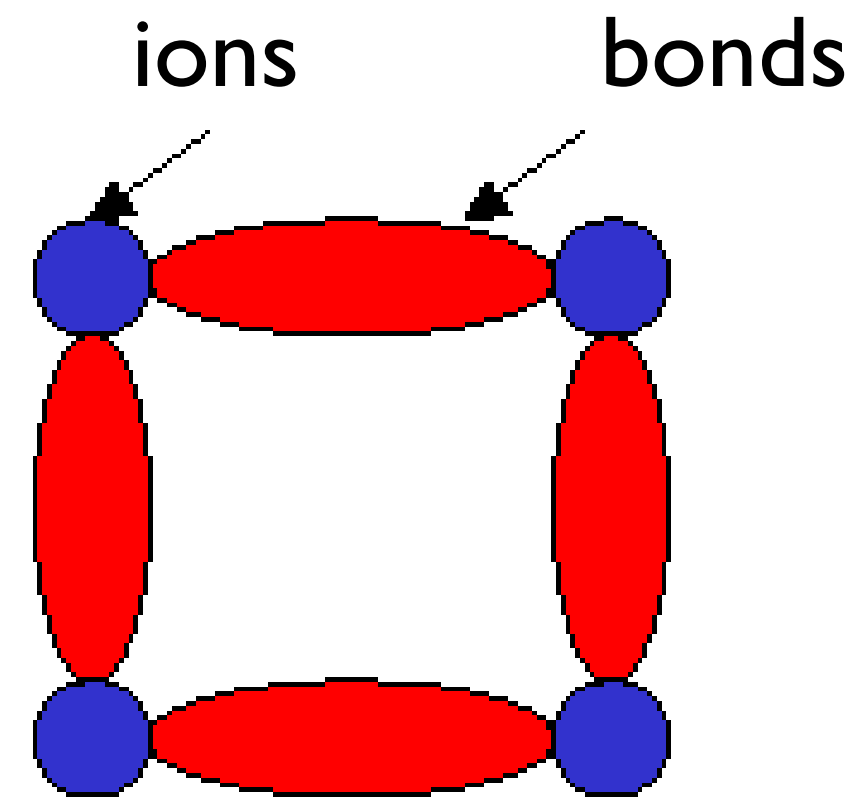


- Structural properties (mechanical properties, crystal structure, surfaces...)
- Electrical properties (resistivity, conductivity, I/V characteristics, Hall effect)
- Thermal properties (specific heat, thermal conductivity)
- Optical properties (color, response to EM fields)

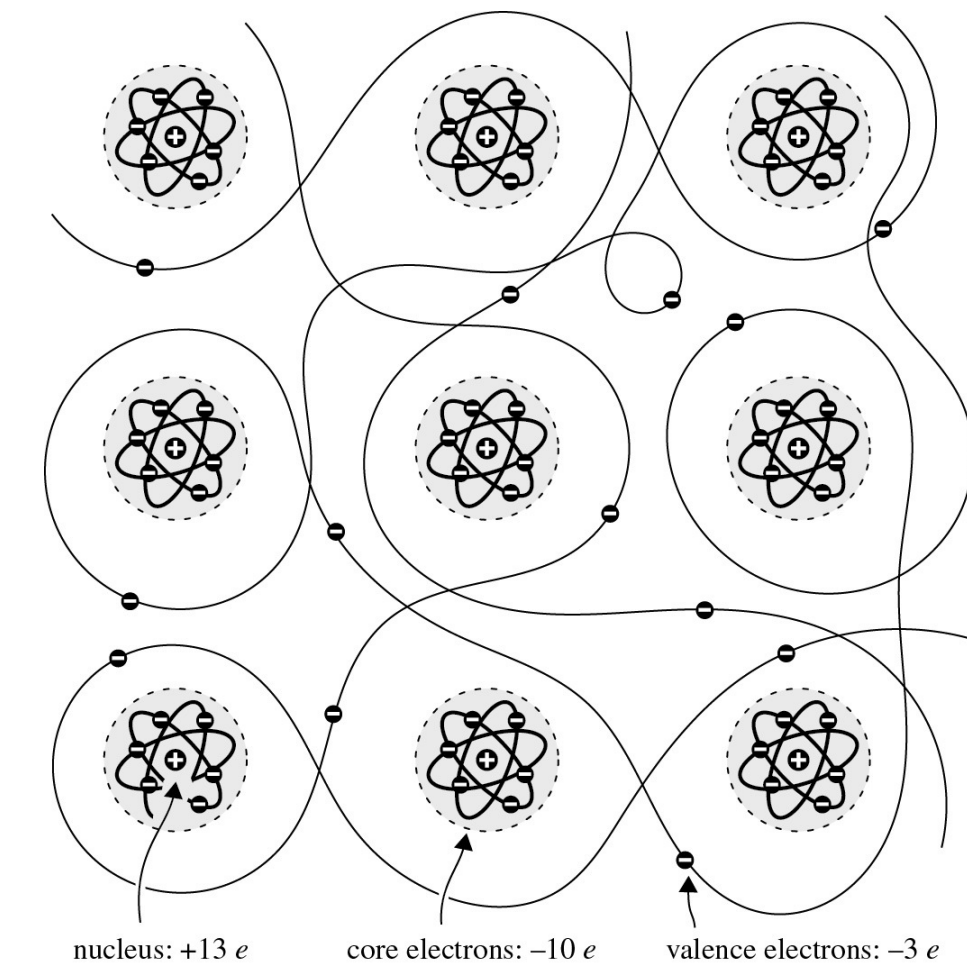
Bonding properties of solids: How much of the individual atom is kept?



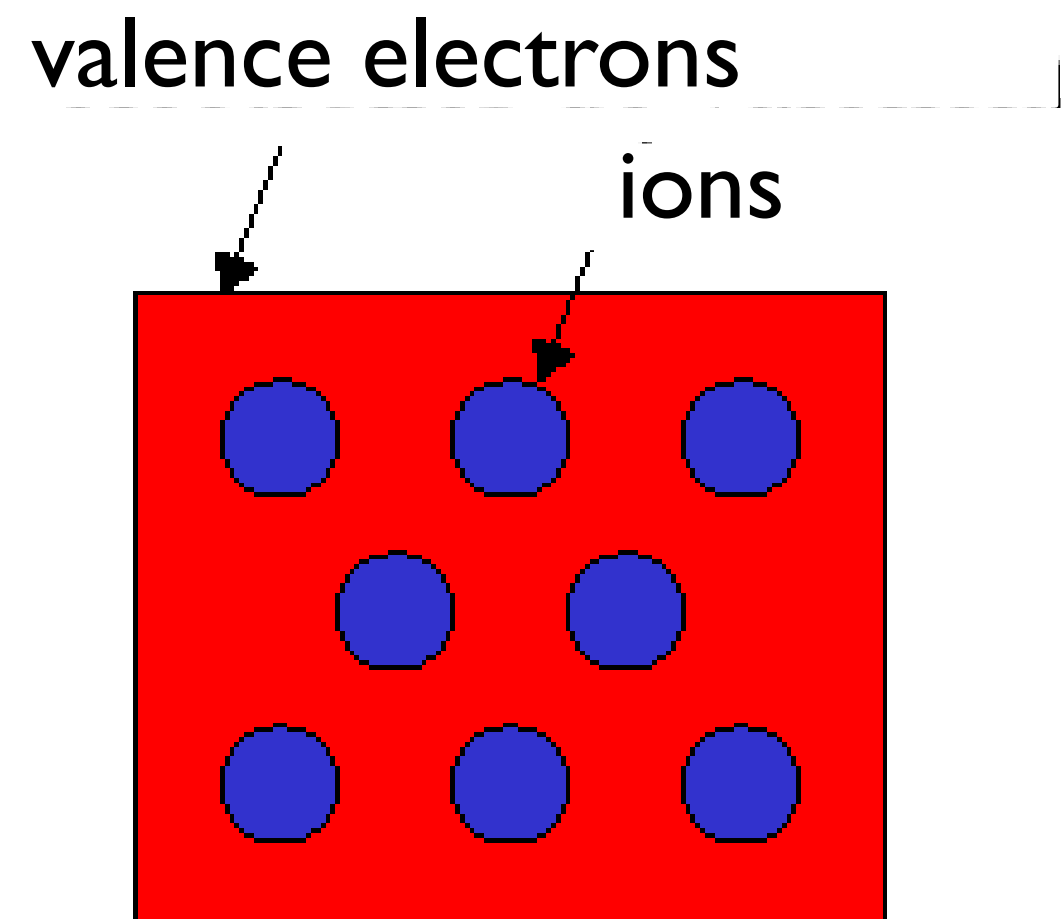
Ionic



Covalent

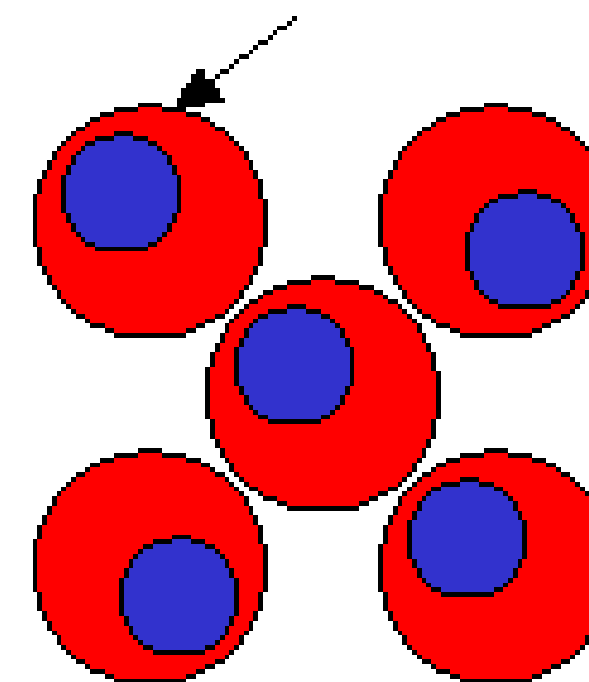


MarvinCohen_Fig.1.1



Metallic

Polarizable atoms



Molecular

Just considering electrical properties there is a huge variation

Solid	Resistivity
Insulator	$10^{14}-10^{22} \Omega\text{cm}$
Semiconductor	$10^{-2}-10^8 \Omega\text{cm}$
Metal	$10^{-6} \Omega\text{cm}$
Superconductor	0

} 28 orders
of
magnitude!!

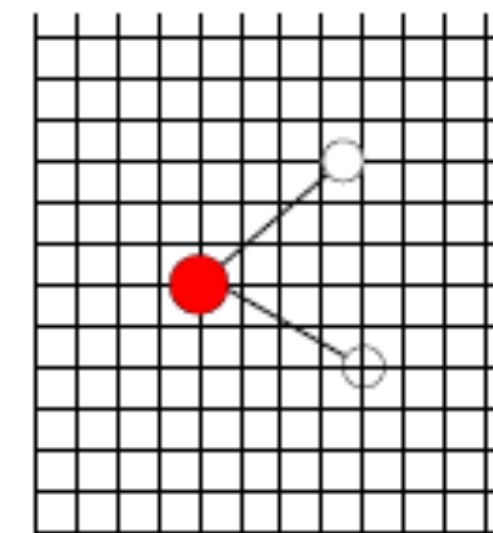
Well, we can use a theory of everything, we know the equation for it!

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

Ground-state energy (without E_{ionic}): $E_0 = \langle \psi_0 | H | \psi_0 \rangle$ with:

- $\psi_0 = \psi_0[r_1\sigma_1, \dots, r_N\sigma_N]$ antisymmetric
- $|\psi_0[r_1\sigma_1, \dots, r_N\sigma_N]|^2 dr_1 \dots dr_N$ probability of finding electron i in $[r_i, r_i + dr_i]$.
- $n(r) = \rho(r) = \langle \psi_0 | \sum_i \delta(r - r_i) | \psi_0 \rangle$ charge density
- $\rho_2(r, r') = \langle \psi_0 | \sum_{i \neq j} \delta(r - r_i) \delta(r' - r_j) | \psi_0 \rangle$ density of pairs, etc.

Problem: We don't know ψ_0 ! We could use variational principle. However with $\psi = \psi[r_1\sigma_1, \dots, r_N\sigma_N]$, calculating $\langle \psi | H | \psi \rangle$ would require $(ngrid)^{3N} \sim 10^{30}$ operations (for small molecule). With 10^{12} flops machine \implies centuries.



Note 2018: tera, peta, exa... 10^{18} ... still years for realistic systems.

“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

Elementary excitation model

Description of solids in the elementary excitation model:

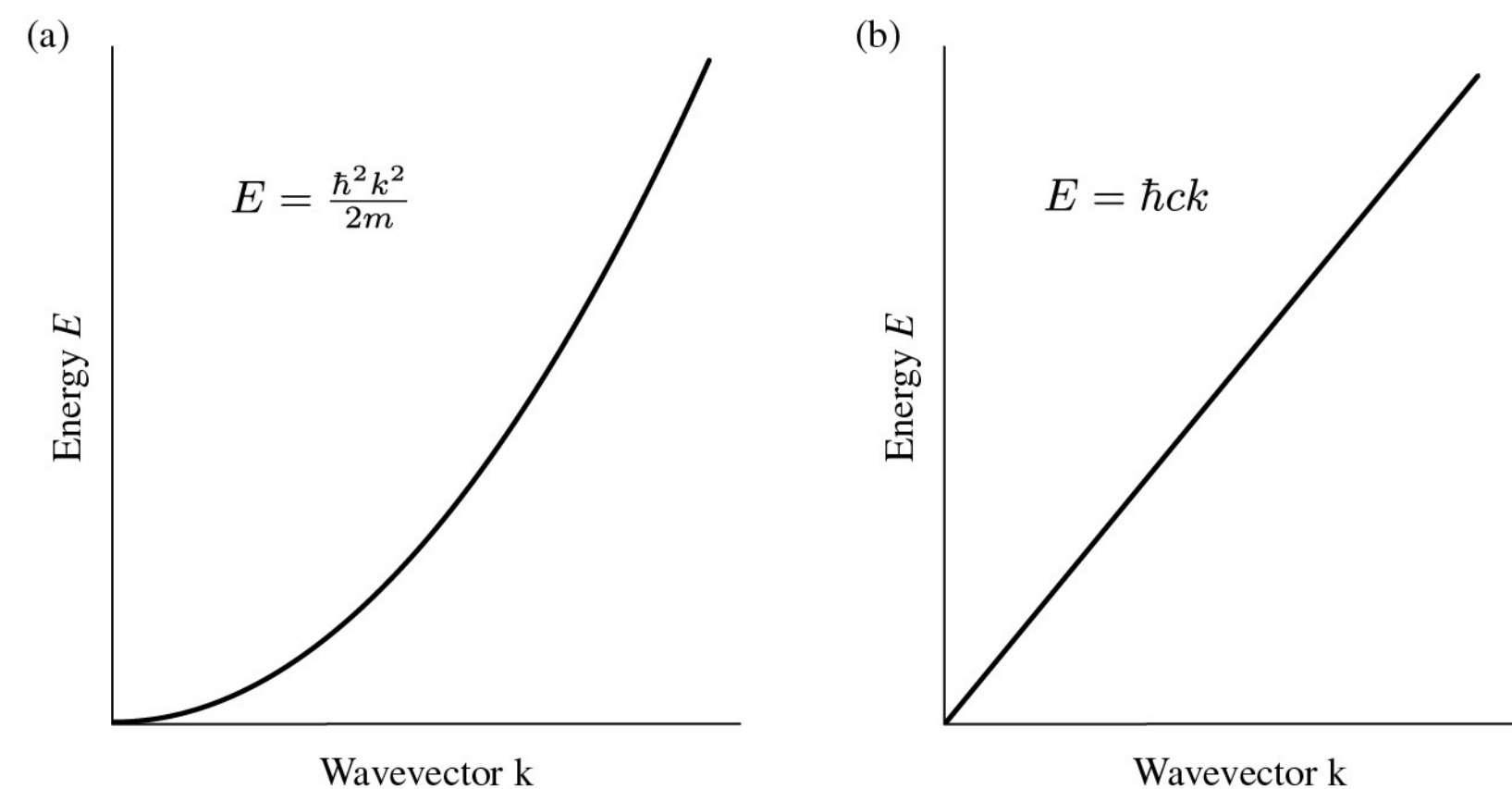
Excitations can emerge when the system is not in the ground state. We need to know the energy spectrum and the density of states (i.e statistics of the system, fermions or bosons)

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

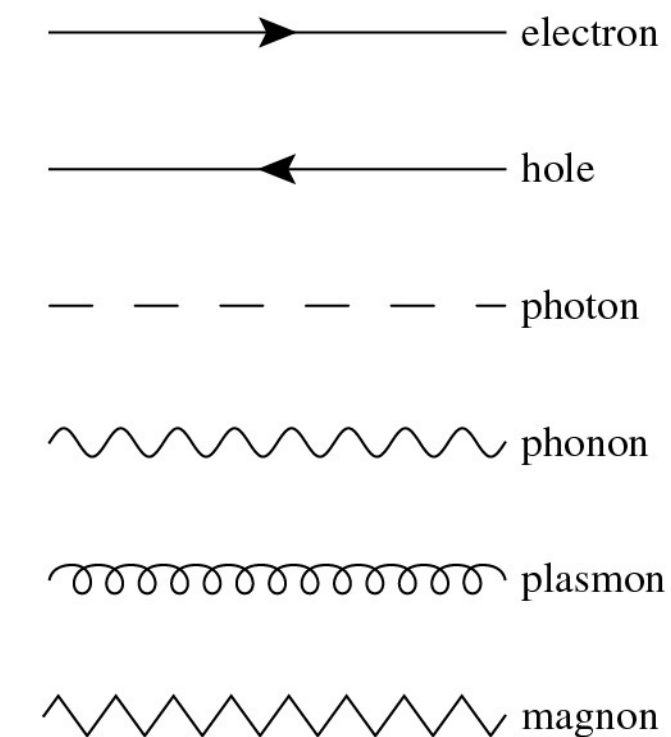
Collective excitations (usually bosons): very different from the underlying particles excitations.

Generalized harmonic oscillators (2nd Quantization)



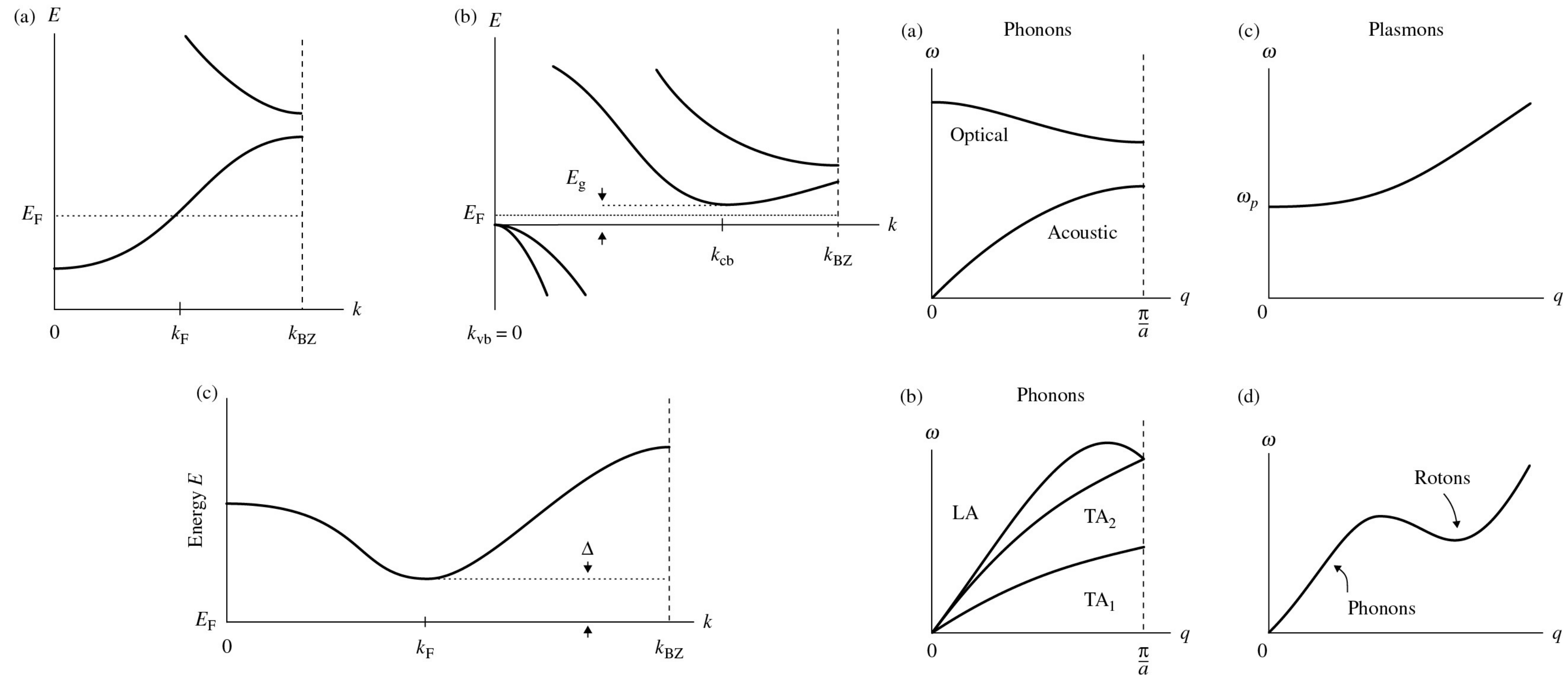
Quasiparticles

- **Quasielectrons:** or electrons. Particles that behave like non-interacting electrons in low lying excited states. Fermions. Ex. Electrons in solids (mass renormalization of free electron). Typical excitation energies are of the order of coulomb energy of 2 e on a lattice of lattice parameter a ($e^2/a \sim 5$ eV). typical $v \sim (e^2/am)^{1/2} \sim 10^8$ cm/s
- **Hole:** opposite charge of a quasielectron
- **Phonon:** Collective excitation of the lattice (boson). wave vector q , polarization mode and energy $\hbar\omega$. Energies of order of $K_b T_D$ (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: $\hbar\omega_p \sim 10$ eV for metals but can be much smaller if electron density n is small ($\hbar\omega_p = \hbar(4\pi ne^2 / m)^{1/2}$)
- **Magnon:** Collective excitation of spins (spin waves). Energies of ~ 0.0001 eV, but can be as high as 0.1 eV)
- **Polaron:** Type of quasielectron Electron+lattice deformation. Very heavy electron. Can be thought as a phonon dressed electron. Binding energies ~ 10 -100 meV
- **Exciton:** Bound state of a quasielectron 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 $\sim T_c \sim 10^{-5}$ - 10^{-2} eV

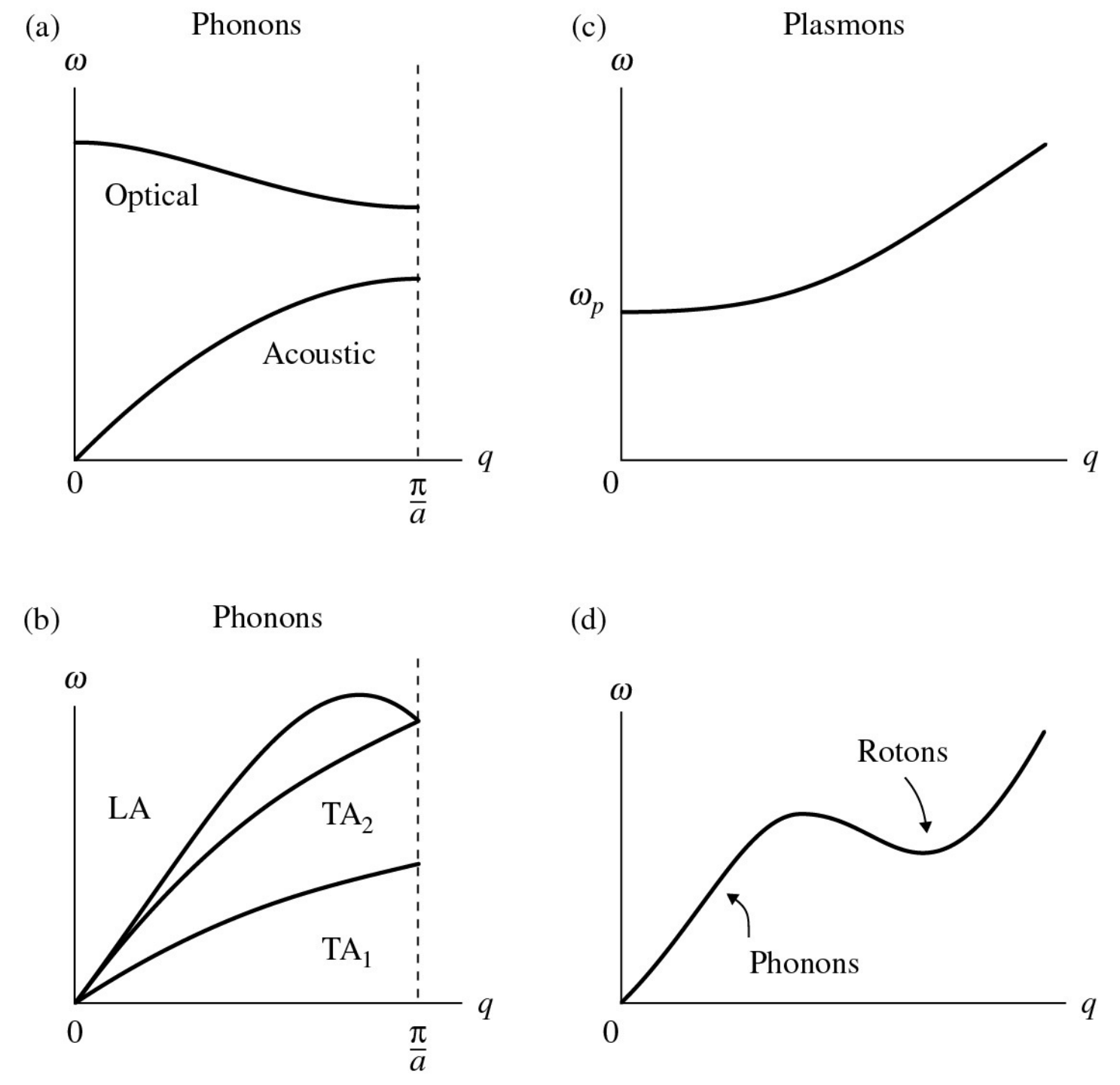


MarvinCohen_Fig.1.5

Dispersion curves

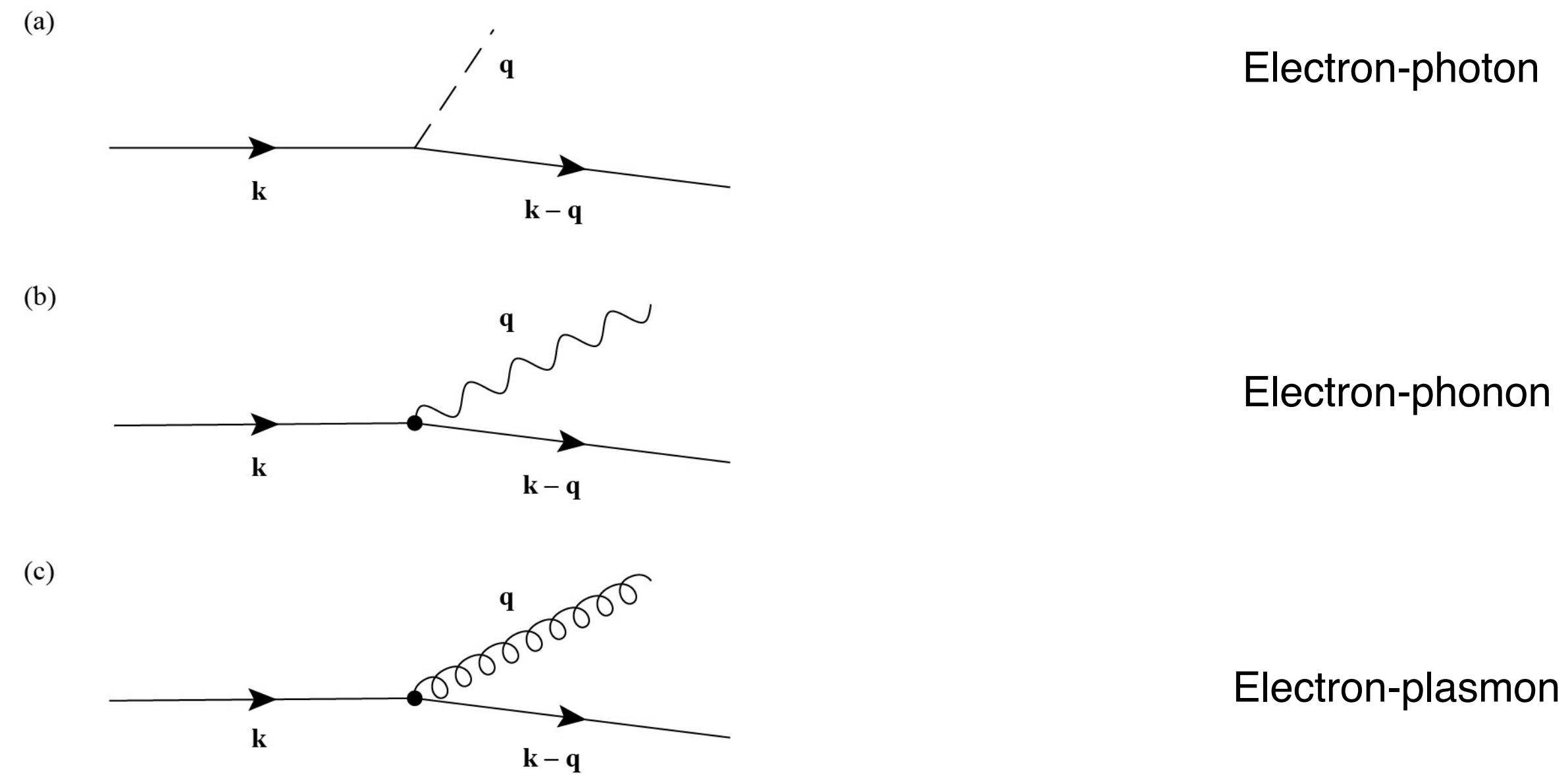


MarvinCohen_Fig.1.3



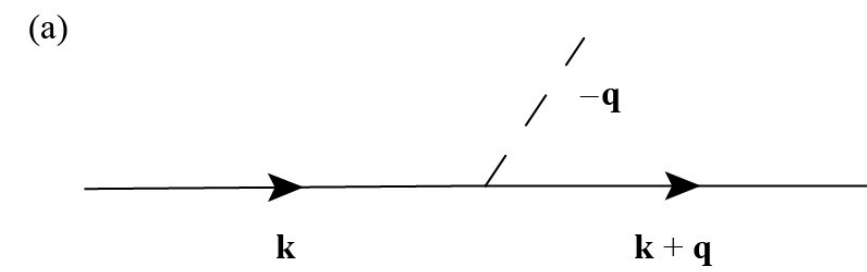
MarvinCohen_Fig.1.4

Interactions among quasiparticles: quasiparticle-boson

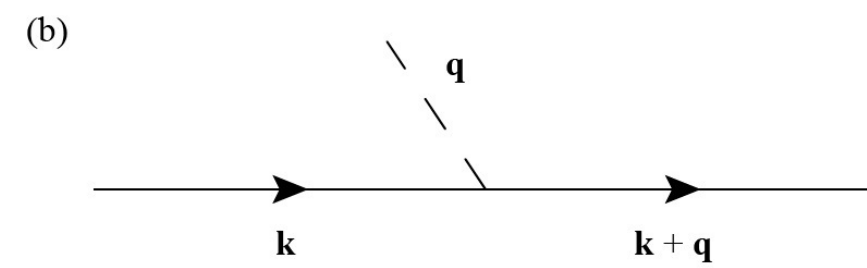


MarvinCohen_Fig.1.7

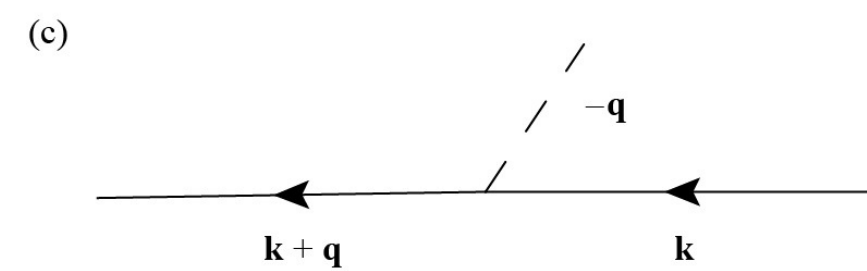
Interactions among quasiparticles: quasiparticle-boson



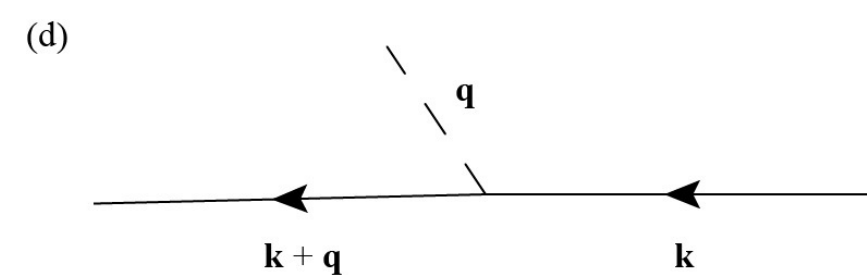
Electron (k) emits a photon ($-q$) scattering into $k+q$



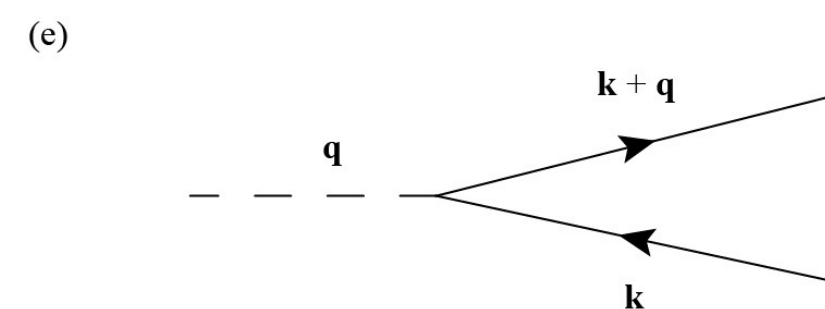
Electron (k) absorbs a photon (q) scattering into $k+q$



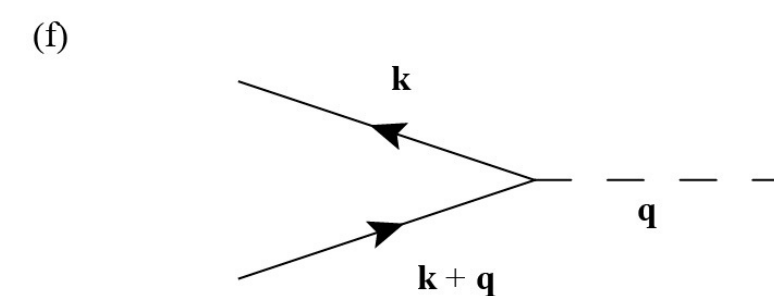
Hole ($-k-q$) emits a photon ($-q$) scattering into $-k$



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

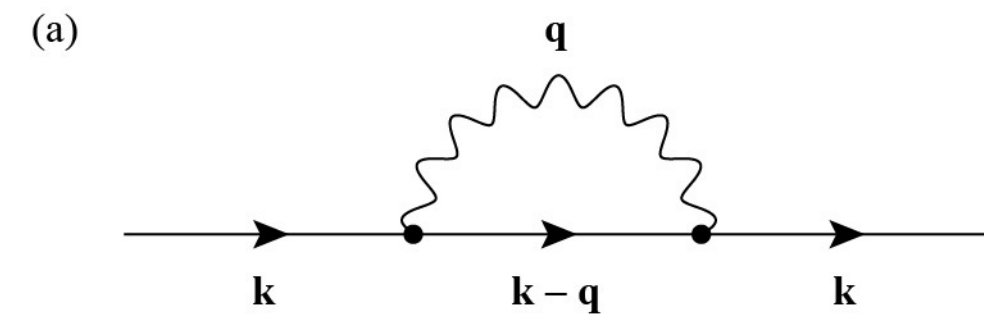


photon (q) creates an electron $k+q$ and hole $-k$

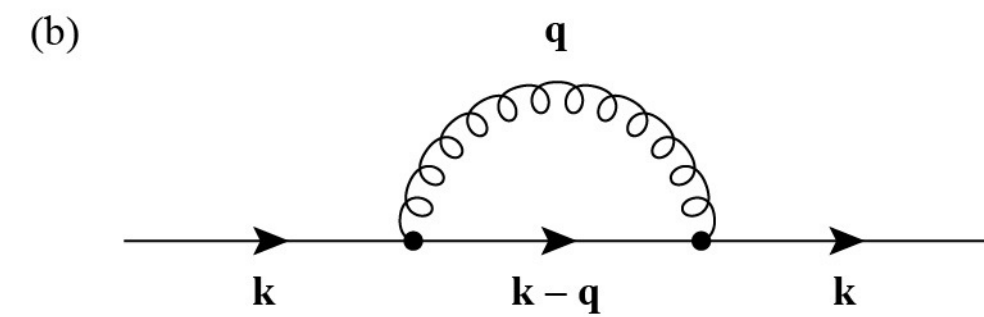


electron ($k+q$) and hole ($-k$) recombine or annihilate into photon (q)

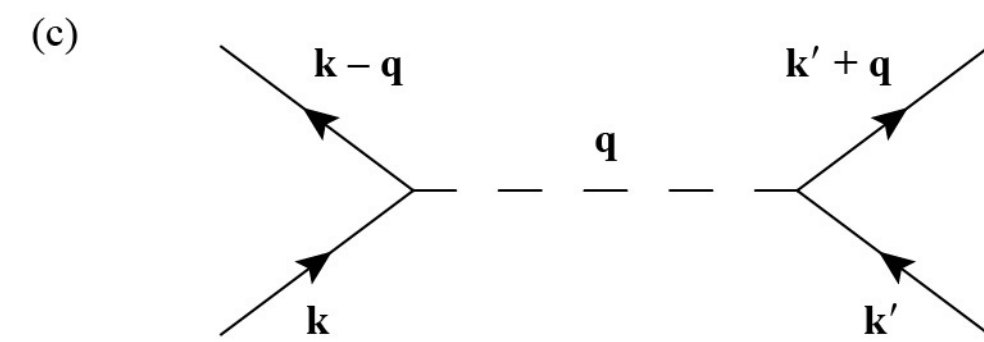
Interactions among quasiparticles: quasiparticle-quasiparticle interactions



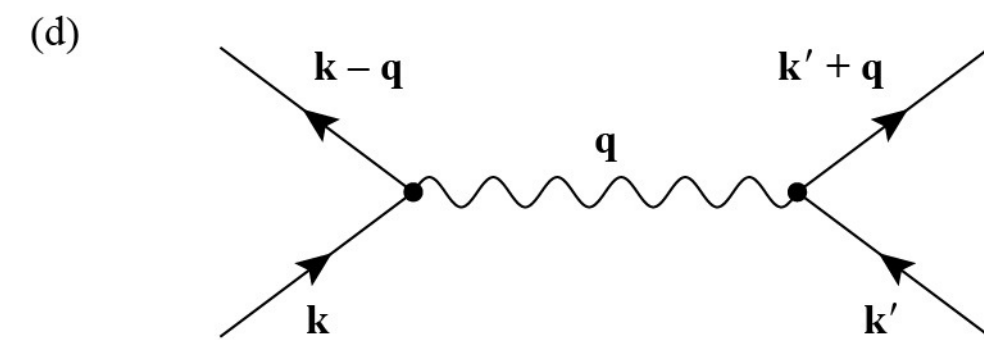
Electron self energy (k) emits and absorbs a phonon (q)



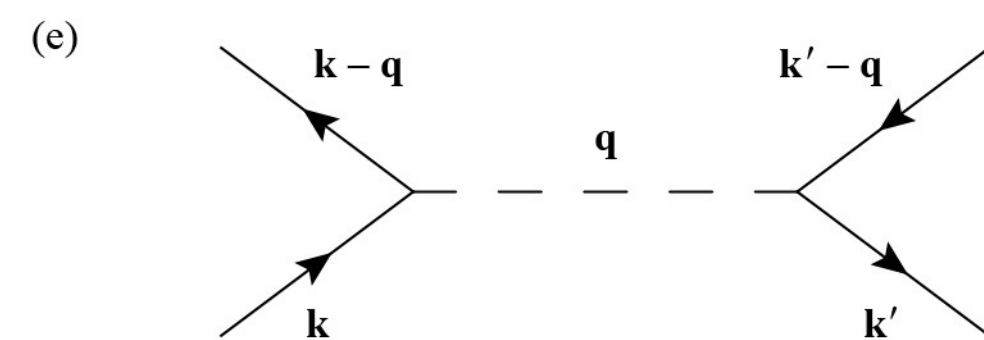
Electron self energy (k) emits and absorbs a plasmon (q)



Electron-electron Coulomb interaction or photon exchange

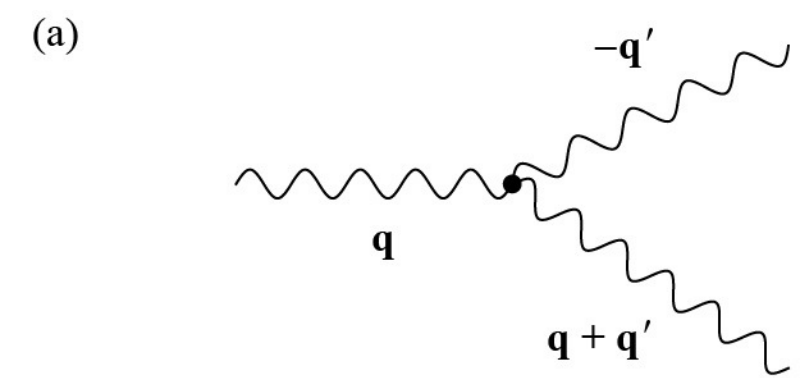


Electron-electron interaction via phonon exchange

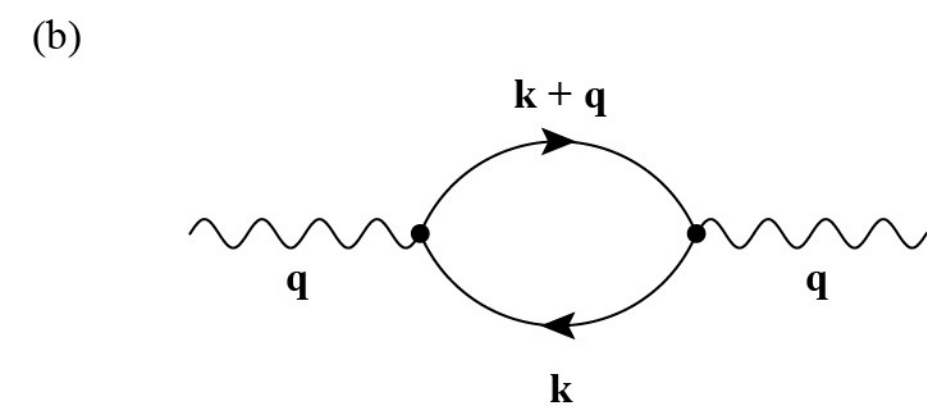


Electron-hole Coulomb interaction

Interactions among quasiparticles: collective excitation interactions



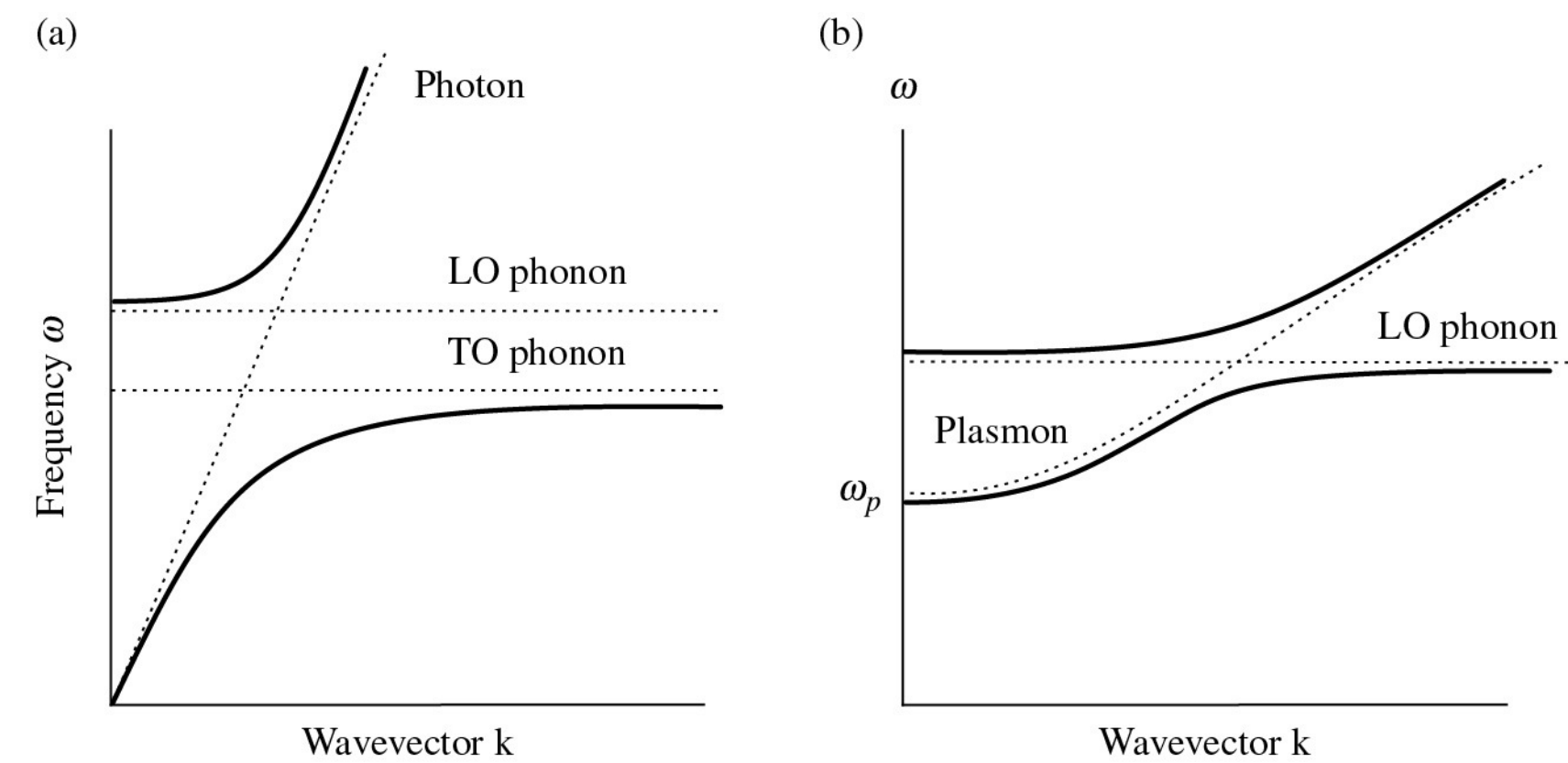
phonon-phonon scattering



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) $M \gg m$ (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.

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

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

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

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

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

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

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.

$M \sim 10^4$ 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

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

$$\hat{H}_{\{\vec{R}_\alpha\}}^{el} \Psi_{n,\{\vec{R}_\alpha\}}^{el}(\{\vec{r}_i\}) = E_n^{el} \Psi_{n,\{\vec{R}_\alpha\}}^{el}(\{\vec{r}_i\})$$

Nuclei

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

Classical dynamics

$$\vec{F}_\alpha = -\frac{\partial E_n^{el}(\{\vec{R}_\mu\})}{\partial \vec{R}_\alpha}$$