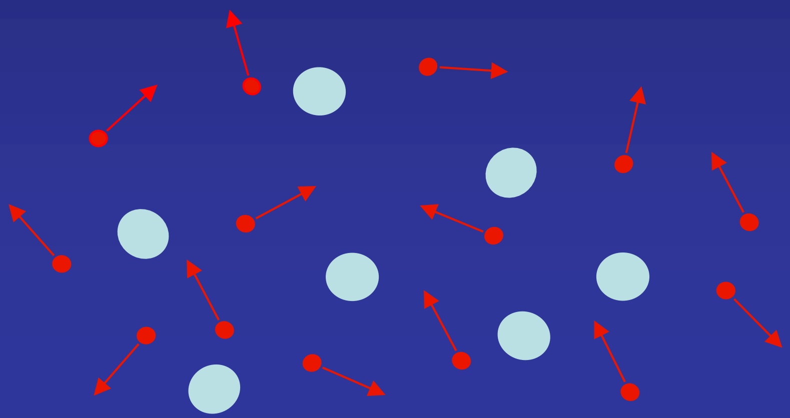
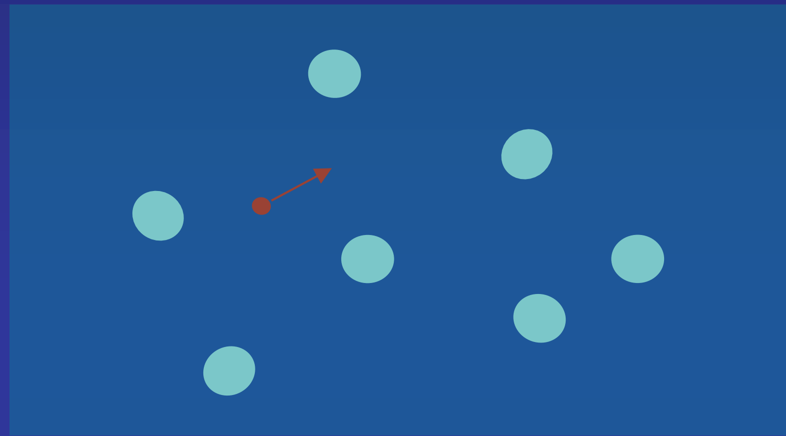
The one electron approximation





Javier Junquera

UNIVERSIDAD DE CANTABRIA

CITIMAC

Basic references, where most of the information is taken from

Harald Ibach and Hans Lüth
"Solid-State Physics"
Springer-Verlag, Berlin, 1993
ISBN 3-540-56841-7

Chapter 6.0

The Hamiltonian of the solid

Solid: combination of:

- **ions (lattice of paticles positively charged and arranged periodically; latt)**
- **electrons (el)**

$$\hat{H}_{\mathrm{solid}} = \hat{H}_{\mathrm{latt}} + \hat{H}_{\mathrm{el}} + \hat{H}_{\mathrm{el-latt}}$$

Phononic states:

VIBRATIONAL PROPERTIES
(heat…)

Electronic states:

ELECTRONIC PROPERTIES

The electron Hamiltonian after the Born-Oppenheimer approximation

All the physics of the system can be described from its Hamiltonian

$$\hat{H}^{\mathrm{el}}_{\{\vec{R}_\alpha\}} = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{1}{4\pi\epsilon_0}\frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{i,\alpha}\frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e^2}{|\vec{r}_i - \vec{R}_\alpha|}$$

Kinetic energy of the electrons

Captures the electron-electron interaction

Coulomb-like Repulsive

Captures the electron-lattice (or electron-phonon) interaction

Coulomb-like Attractive

To solve the electronic problem within the adiabatic or Born-Oppenheimer approximation, one can regard the nuclear or core motion as nonexistent

To know the steady-state electronic wave function and the energy of the electronic subsystem, we need to solve the time-independent Schrödinger equation

$$\hat{H}^{\mathrm{el}}_{\{\vec{R}_\alpha\}}\Psi^{\mathrm{el}}_{n,\{\vec{R}_\alpha\}} = E_n^{\mathrm{el}}\Psi^{\mathrm{el}}_{n,\{\vec{R}_\alpha\}}$$

n **is a Quantum index of the system**

The nuclear positions are taken as fixed parameters.

Ψ does not depend on the temporal vibration of the nuclei

Problem: how to solve the Schrödinger equation for the electronic subsystem

$$\hat{H}^{\mathrm{el}}_{\{\vec{R}_\alpha\}} \Psi^{\mathrm{el}}_{n,\{\vec{R}_\alpha\}} = E^{\mathrm{el}}_n \Psi^{\mathrm{el}}_{n,\{\vec{R}_\alpha\}}$$

Solve it for:

- **About 10^{23} electrons**
- **That interact one with another**
- **In a periodic, static core potential**

An overwhelming, exceedingly difficult problem

One electron approximation

We shall consider the movement of :

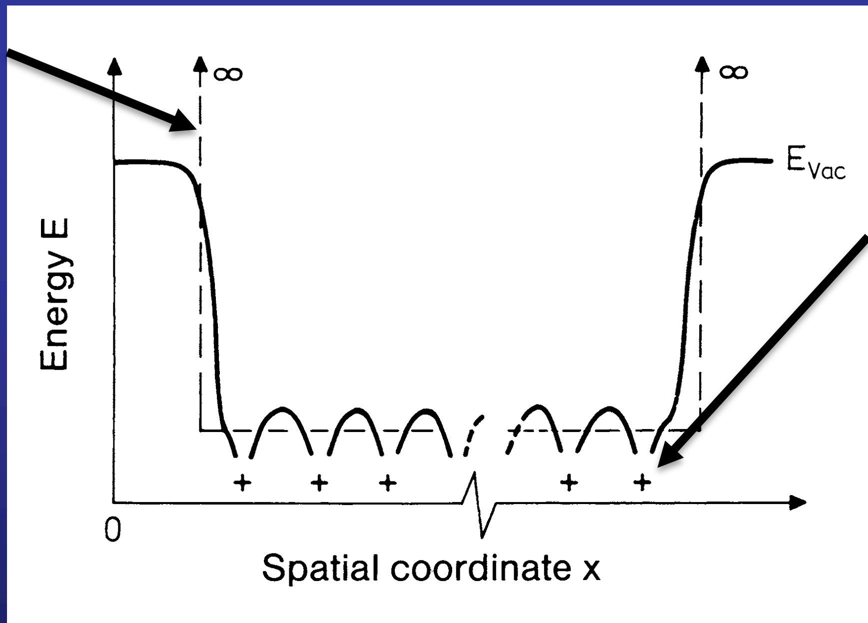
a simple electron

in an effective periodic and time independent potential

The potential is the one produced by:
- The stationary nuclei in their equilibrium positions
- By all the other electrons

Surface of the cristal, generates a potential energy barrier.

E_{Vac} is the energy level to which electron must be promoted in order to leave the crystal



From Ibach and Lüth

Potential due to the atomic nuclei (shape of a well).
Nuclei are periodically distributed in the stationary equilibrium positions

These nuclei are surrounded by the electrons of the inner shells, that will screen the nuclear potential

One electron approximation: limits of applicability

We shall neglect all electron-electron interactions that cannot be represented as a local potential for the single electron

For example:

- Exchange interaction $\Longrightarrow$ No magnetism
- Long distance electronic correlations
- Coupling of electrons in pairs $\Longrightarrow$ No superconductivity

One electron approximation shall be considered from now on, unless otherwise stated

From now, we shall asume a local periodic potential

We shall solve the Schrödinger equation for a single electron

The corresponding quantum states will be filled according with electrons according to the Pauli principle (electrons are Fermions)
Each state will contain only a single electron
(two with opposite spins if we consider the spin degeneracy)