Band theory of solids

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Electronic energies in solids

In solids, since many atoms interact, permissible electron energies occur in bands.

Two approaches to see the origin of energy bands:

Isolated atom approach: generalize the idea of level splitting from covalent bonds to splitting by many atoms.

Lattice wave function: show that wave function of crystal lattice yields energy bands.

Isolated-atom approach

Suppose the wave function for an isolated electron around atom 1 is ψ_1, and that for an isolated atom around atom 2 is ψ_2.

If we bring the atoms close enought to interact, we must consider the combined wave functions

$$\psi_1 + \psi_2 \text{ and } \psi_1 - \psi_2$$

This splits the energy levels—the bonding state has a lower E, the antibonding a higher E. There is a splitting of ΔE.

ΔE depends on the number of atoms close enough for strong interaction, so it is small.

There is a band for every electronic energy level of the atom, but most are full. For each atom in the solid there is one level—a band of $N \sim 10^{23}$ levels each a tiny ΔE apart.

In Na, the $3s$ band can hold $2N$ electrons/level, but each Na only has one—the band is half full.

Conduction in metals

E_F lies *within* the conduction band.

If an $\vec{\mathbf{E}}$ field is applied to a metal, electrons near E_F can gain energy from the $\vec{\mathbf{E}}$ field and reach nearby empty energy states—thus they are free to move among the unoccupied states—conduction.

In insulators

A lower (valence) band is completely filled. The next higher electronic state in an atom is an energy gap $E_g \sim 10$ eV higher and makes the conduction band. $E_g \gg k_B T$, and E_F is about the midpoint of the *gap*. FD statistics says very few electrons will reach the conduction band at $T \sim 300$ K. Hence the material has a high resistivity.

Semiconductors

The energy gap is smaller $E_g \sim 1$ eV. This is small enough that some electrons reach thermal energies to cross the gap at room T.

There are many states available in the conduction band, so an $\vec{\mathbf{E}}$ field can cause conduction of electrons.

Also, in the valence band, the electrons leave valence sites empty, which act as**holes**—carriers of charge $+e$. A semiconductor that has these when pure is an **intrinsic semiconductor.**

Charge carriers in semiconductors can be modified by adding other atoms—**doping.**

Next topic: semiconductors and the $p-n$ junction.

Recommended website for QM simulations:

`www.falstad.com/mathphysics.html`