Gibbs sum: Donor level and acceptor level in semiconductor

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1. Occupancy of donor

A donor level can be occupied by an electron with either spin up or spin down. Once the level is occupied by one electron, the donor cannot bind a second electron with opposite spin. We suppose that one, but only one, electron can be bound to an impurity atom, either orientation $\uparrow$ or $\downarrow$ of the electron spin is accessible. The possible microscopic states for a donor level are the empty state, the state occupied by an electron of spin up and that of spin down.
The Gibbs sum is given by

$$Z_G = 1 + 2ze^{-\beta E_d}$$

The probability that the system is ionized ($N = 0$) is

$$P(\text{ionized}) = f(D^+) = \frac{1}{Z_G} = \frac{1}{1 + 2ze^{-\beta E_d}} = \frac{1}{1 + 2e^{\beta(\mu - E_d)}}$$

The probability that the system is neutralized is

$$P(\text{neutral}) = f(D) = 1 - \frac{1}{1 + 2ze^{-\beta E_d}} = \frac{2ze^{-\beta E_d}}{1 + 2ze^{-\beta E_d}} = \frac{1}{1 + \frac{1}{2}e^{\beta(E_d - \mu)}}$$

Note that two electrons with opposite spins are not allowed in the same site because of the repulsive Coulomb interaction. The factor 2 is the spin degeneracy.

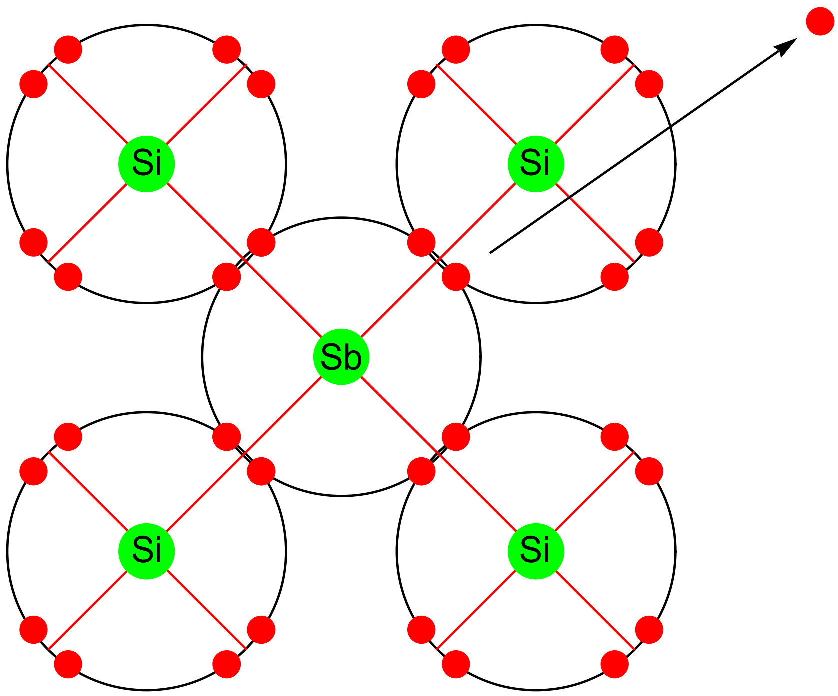

Fig. *N*-type semiconductor with donor level.

2. Occupancy of acceptor

In the ionized condition A^- of the acceptor, each of the chemical bonds between the acceptor atom and the surrounding semiconductor Si atoms, contains a pair of electrons with antiparallel spins. There is only one such state.

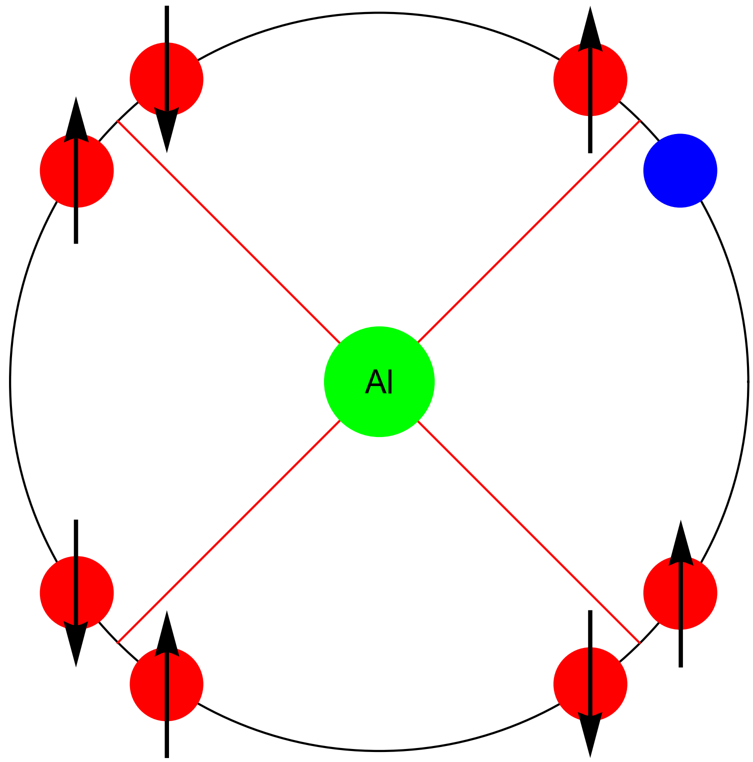

Fig. The spin direction is fixed.

In the above figure, the electron in the spin down state.

1. $1\, ze^{-\beta\varepsilon_a}$: one electron with spin down

In the neutral condition A of the acceptor, one electron is missing from the surrounding bonds. The missing electron may have either spin up or spin down.

2. one $\uparrow$ electron missing ($N = 0$, zero energy)
3. one $\downarrow$ electron missing ($N = 0$, zero energy)

Thus we have the partition function

$$Z_G = 2 + ze^{-\beta\varepsilon_a}.$$

$$f(A^-) = \frac{ze^{-\beta\varepsilon_a}}{2 + ze^{-\beta\varepsilon_a}} = \frac{1}{\frac{2}{z}e^{\beta\varepsilon_a} + 1} = \frac{1}{1 + 2e^{\beta(\varepsilon_a - \mu)}}$$

(the acceptor orbital occupied)

$$f(A) = \frac{2}{2 + ze^{-\beta\varepsilon_a}} = \frac{1}{1 + \frac{1}{2}e^{\beta(\mu - \varepsilon_a)}}$$

(the acceptor orbital unoccupied)

3. Summary

The electron concentrations in the donner level and the acceptor level ar

$$n_D = N_d f(D) = \frac{N_d}{1 + \frac{1}{2}e^{\beta(E_d - \mu)}}$$

$$n_A = N_A f(A^-) = \frac{N_A}{1 + 2e^{\beta(\varepsilon_a - \mu)}}$$