Spin statistic. Case of a Non-magnetic metal

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main idea: The electron distribution depends on occupancy of a quantum state (single or double occupancy) by a conduction electrons. The distributions of electrons single- or double occupancy are calculated from a balance of scattering rates between these two groups of electrons.

The electron is an elementary particle and a fermion. It makes some restriction, which greatly influence the electron and hole transport

(quantum nature of electron) (restriction 1): The energy distribution of electrons is the Fermi- Dirac distribution.

(quantum nature of electron) (restriction 2): Each conduction electron occupies one quantum state. Each quantum state can be occupied by one or two conduction electrons

(quantum nature of electron) (restriction 3): The electron can change its energy (e.g. in an electrical field) or movement direction only if the corresponded quantum state is unoccupied and available for the electron to be scattered into.

(quantum nature of electron) (restriction 4): The conduction electron can be scattered in a quantum state, which is already occupied by one electron, only when its spin is opposite to the spin of the already- existing electron

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A quantum state of conduction electrons can be occupied either by two, one or none electrons. Depending on occupancy number, the electron distribution is slightly different. Therefore, all conduction electron and corresponded quantum states can be divided into 3 groups:

(*group 1*) quantum states occupied by two electrons. These states are called "**full**" and electrons are **spin-inactive**. Spins of electrons in this group are distributed equally in all directions.

(*group 2*) quantum states occupied by a single electron. These groups of conduction electrons are **spin-unpolarized** (old name is TIS).

(*group 3*) unoccupied quantum states. These states are called "**empty**"

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The electrons are constantly scattered between different groups. In equilibrium, the number of electrons in each group does not change. Therefore, there is a balance between scattering rates between different groups.

There are 4 possible scattering events and 2 of them do change the number electrons in the groups.

Scattering events, which **do not change** number of electrons in group

(*scattering event 1*): scattering of an electron from a single- occupied state into an unoccupied state (an "empty" state). The result of the scattering is one single- occupied state and an "empty" state. It is the same types of states, which were before scattering.
(*scattering event 2*): scattering of an electron from a double- occupied state (a "full" state) into an a single- occupied state The result of the scattering is one single- occupied state and an "full" state. It is the same types of states, which were before scattering.

Scattering events, which **change** number of electrons in group

(*scattering event 3*): scattering of an electron from a double- occupied state (a "full" state) into an unoccupied state (an "empty" state). The result of the scattering is two single- occupied states with electrons with opposite spins. The scattering reduces number of "full" and "empty" states and increases the number of single-occupied states.

(*scattering event 4*): scattering of an electron from a single- occupied state The result of the scattering is a double- occupied state (a "full" state) into an unoccupied state (an "empty" state). The scattering reduces the number of single-occupied states and increases number of "full" and "empty" states.

Scattering Influence of electron spin on the scatterings

The scattering events 1, 2 and 3 are not influence by electron spin.
As a result, the rate of the scattering event 3 is calculated as

$$\frac{\partial n_{TIS}}{\partial t} = 2 \cdot n_{full} \cdot n_{empty} \cdot p_{scat} \quad (1)$$

$$\frac{\partial n_{full}}{\partial t} = \frac{\partial n_{empty}}{\partial t} = -n_{full} \cdot n_{empty} \cdot p_{scat} \quad (2)$$

where n_{TIS}, n_{full}, n_{empty} is the number of single-occupied, double- occupied and unoccupied states, correspondently. p_{scat} is the probability of an electron scattering event per unit time. The 2 is used because the result of the scattering is two single- occupied states.

The scattering event 4 is spin- dependent. The electron from a single- occupied state can be scattered into another single- occupied state only if its spin direction is opposite to the electron spin in that state. It reduces the scattering probability. The scattering event 4 and increases number of "full" and "empty" states.. Therefore, the rate of the scattering event 3 is calculated as

$$\frac{\partial n_{full}}{\partial t} = \frac{\partial n_{empty}}{\partial t} = p_{spin} \cdot n_{TIS} \cdot n_{TIS} \cdot p_{scat} \quad (3)$$

$$\frac{\partial n_{TIS}}{\partial t} = -2 \cdot p_{spin} \cdot n_{TIS} \cdot n_{TIS} \cdot p_{scat} \quad (4)$$

where p_{spin} is the probability that spins of electrons in two single- occupied states are in opposite directions. The p_{spin} can be calculated (See Appendix) as

$$p_{spin} = 1 - \frac{\pi^2}{16} \approx 0.1916 \quad (5)$$

The balance of the scattering rates. In equilibrium, the number of electrons in each group does not change. From Eqs. (1) and (4) or (2) and (3), the balance is obtained as

$$2 \cdot n_{full} \cdot n_{empty} = p_{spin} \cdot n_{TIS}^2 \quad (6)$$

The Fermi-Dirac distribution. The energy distributions of electrons are described by the Fermi-Dirac statistic. The probability for a conduction electron to occupy a quantum state is calculated as

$$p_e(E) = F_{Fermi-Dirac} = \frac{1}{1+e^{\frac{E-E_F}{kT}}} \quad (7)$$

where E_F is the Fermi energy

The probability that a quantum state is not occupied by a conduction electron is calculated as

$$p_h(E) = 1 - F_{Fermi-Dirac} = 1 - \frac{1}{1+e^{\frac{E-E_F}{kT}}} \quad (8)$$

Calculation of energy distribution for each group of electrons

Each "full state is occupied by two electrons and one electron is in a single- occupied state. The probability of for an electron to occupy a quantum state (Eq.7) is calculated as

$$p_e(E) = 2 \cdot p_{full}(E) + p_{TIS}(E) = F_{Fermi-Dirac}(E) \quad (9)$$

There are two unocupied places in a empty state and one place in a single- occupied state. The probability that a quantum state is not occupied by a conduction electron (Eq.7) is calculated as

$$p_h(E) = 2 \cdot p_{empty}(E) + p_{TIS}(E) = 1 - F_{Fermi-Dirac}(E) \quad (10)$$

where p_{TIS}, p_{full}, p_{empty} is the probability of single-occupied, double- occupied and unoccupied states, correspondently.

Eq.6 gives

$$2 \cdot p_{full} \cdot p_{empty} = p_{spin} \cdot p_{TIS}^2 \quad (6a) \quad \text{with} \quad p_{spin} = 0.5\left(1 - \frac{\pi^2}{16}\right) \approx 0.1916 \quad (5)$$

From Eqs 9 and 10

$$2 \cdot p_{full} = F_{Fermi-Dirac} - p_{TIS} \quad (9a)$$

$$2 \cdot p_{empty} = 1 - F_{Fermi-Dirac} - p_{TIS} \quad (10a)$$

Substitution of Eqs. 9a and 10a into Eq. 6a gives

$$(F_{Fermi-Dirac} - p_{TIS}) \cdot (1 - F_{Fermi-Dirac} - p_{TIS}) = 2 \cdot p_{spin} \cdot p_{TIS}^2 \quad (11)$$

Simplifying Eq. (11) gives

$$(1 - 2 \cdot p_{spin}) \cdot p_{TIS}^2 - p_{TIS} + F_{Fermi-Dirac} \cdot (1 - F_{Fermi-Dirac}) \quad (12)$$

The solution of the quadratic equation (12) is

$$p_{TIS}^2 - 2c \cdot p_{TIS} + 2c \cdot F_{Fermi-Dirac} \cdot \left(1 - F_{Fermi-Dirac}\right) \quad (12)$$

where $c = \frac{1}{2} \frac{1}{1 - 2 \cdot p_{spin}} = \frac{8}{\pi^2} \approx 0.8106$

the solution of the quadratic equation (12) is

$$p_{TIS} = c \pm \sqrt{c^2 - 2c \cdot F_{Fermi-Dirac} \cdot \left(1 - F_{Fermi-Dirac}\right)} \quad (13)$$

taking into account only solution with "-" and

$$F_{Fermi-Dirac} \cdot \left(1 - F_{Fermi-Dirac}\right) = \frac{1}{1 + e^{\frac{E-E_F}{kT}}} \left(1 - \frac{1}{1 + e^{\frac{E-E_F}{kT}}}\right) = \frac{e^{\frac{E-E_F}{kT}}}{\left(1 + e^{\frac{E-E_F}{kT}}\right)^2} = \frac{e^{\frac{E-E_F}{kT}}}{1 + 2e^{\frac{E-E_F}{kT}} + e^{2\frac{E-E_F}{kT}}} =$$

$$= \frac{1}{e^{-\frac{E-E_F}{kT}} + 2 + e^{\frac{E-E_F}{kT}}} = \frac{0.5}{1 + \cosh\left(\frac{E - E_F}{kT}\right)}$$

Eq.(13) is simplified as

$$p_{TIS} = c\left[1 - \sqrt{1 - \frac{1}{c} \frac{1}{1 + \cosh\left(\frac{E - E_F}{kT}\right)}}\right] \quad (14)$$

and therefore the probability that a conduction electron occupies a single- occupied state is calculated as

$$\boxed{p_{TIS} = \frac{8}{\pi^2}\left[1 - \sqrt{1 - \frac{\pi^2}{8} \frac{1}{1 - \cosh\left(\frac{E - E_F}{kT}\right)}}\right] \quad (15)}$$

the probability that a conduction electron occupies a double- occupied state (a "full" state) is calculated as

$$\boxed{p_{full} = F_{Fermi-Dirac} - p_{TIS} = \frac{1}{1 + e^{\frac{E-E_F}{kT}}} - \frac{8}{\pi^2}\left[1 + \sqrt{1 - \frac{\pi^2}{8} \frac{1}{1 - \cosh\left(\frac{E - E_F}{kT}\right)}}\right] \quad (16)}$$

the probability of an unoccupied place in "empty" state is calculated as

$$p_{empty} = 1 - F_{Fermi-Dirac} - p_{TIS} = 1 - \frac{1}{1 + e^{\frac{E-E_F}{kT}}} - \frac{8}{\pi^2}\left[1 - \sqrt{1 - \frac{\pi^2}{8}\frac{1}{1+\cosh\left(\frac{E-E_F}{kT}\right)}}\right] \quad (17)$$