Armenian Journal of Physics, 2022, vol. 15, issue 2-3, pp. 101-105

Screened Potential by Electron Gas

A.I. Soghmonyan, S.A. Mkhitaryan*, J.P. Markosyan

DOI:10.54503/18291171-2022.15.2-3-101

Institute of Applied Problems of Physics of the National Academy of Sciences of the Republic of Armenia
25Hrachya Nersisyan Str., 0014, Yerevan, Republic of Armenia
*E–mail: sammkhitar@yahoo.com

Abstract. Donors and acceptors in semiconductors are charged impurities with a Coulomb potential and, therefore, are screened by free charge carriers – electrons. An analytical description of the oscillations of the screened external potential by the electron gas is considered in this paper. Using the inverse transformation of the Fourier component, the screened Coulomb Potential *U(r)* and the value of the screening radius r_s for the degenerate and nondegenerate electron gas are found. The dependence of r_s on potentials is also given. It is shown that the screening radius decreases with increasing the electron density.

Keywords: Coulomb potential, electron gas, screening radius, degenerate and nondegenerate electron gas.

1. Introduction

Quite a lot of effort was lost at one time in the study of the gas of electrons with the Coulomb interaction [1–5]. It is known that an electron cloud that is homogeneous on average undergoes fluctuations in the electron density. The Coulomb field decreases so slowly with distance that the charge fluctuation at a given point in the crystal causes a redistribution of charges even at the most remote points in the gas. Such a distant correlation in the movement of electrons does not allow them to approach too much closely and creates a rarefied cloud of other electrons near each electron.

Neutrality in the crystal is carried out due to positively charged ionic residues. There fore, in the region of a rarefied cloud surrounding each given electron, the positive charge of the ionic remains "shines through". This positive charge compensates the Coulomb electric field of the electron everywhere except for a small neighborhood of the electron. It turns out that two electrons interact only when they are at a very small distance from each other, that is, through a short–range screened potential [1,2].

The complexity of constructing a theory of such a screened potential is that such a theoretical consideration must be self–consistent, that is, one must find a potential that gives such electronic states and charge density that lead to an initial potential. Particular attention is paid to the concept of elementary excitations, which turns out to be very productive in the quantum theory of solids. First of all, the Coulomb interaction of charged current carriers is considered. This interaction determines the screening effects, exciton optical properties, and metal–insulator transitions.

The screening of the Coulomb interaction arises due to fluctuations in the electron density. The screening phenomenon consists in the fact that the ion "gathers" around itself an unevenly charged cloud of mobile charges of the opposite sign. The charge of the cloud is equal in magnitude and opposite in sign to the charge of the ion, and together they create an electrostatic potential *U(r),* where *r* is the radius vector directed from the center of the ion to the screening cloud [3, 4].

2. Theoretical Approaches

In semiconductors, donors and acceptors are charged impurities with a Coulomb potential energy equal to

$$W(r)\sim\frac{e^2}{|r|}, \tag{1}$$

where e is the electron charge, r – radius vector.

Potential energy plays here the role of external potential. In this paper, we consider the screening of this potential by an electron gas. The Fourier component of the impurity Coulomb potential can be obtained by calculating the integral [2]

$$I = \frac{1}{V}\int \frac{1}{|r|} e^{-iqr-\alpha r} d^3 r, \tag{2}$$

in which the $e^{-\alpha r}$ is a factor added to the integrand to ensures good convergence of the integral, V– voiume, q – quasi–wave vector, α – absorption coefficient.

To calculate this integral, it is convenient to use spherical coordinates and represent it in the form

$$I = 2\pi \int r dr \int_{-1}^{+1} dx e^{-i|q|\cdot|r|x-\alpha r} = \frac{2\pi}{-iq}\left\lfloor \frac{1}{i(q-i\alpha)} + \frac{1}{i(q+i\alpha)} \right\rfloor = \frac{4\pi}{q^2+\alpha^2} \tag{3}$$

Assuming the auxiliary quantity α to be equal to zero in (3), we obtain the Fourier component of the Coulomb potential in the form

$$W_q = \frac{4\pi e^2}{q^2}\frac{1}{V} \quad . \tag{4}$$

Impurity potential (1) is static, therefore, when considering the self–consistency condition

$$U(r,t) = W(r,t) + \delta U(r,t), \tag{5}$$

the frequency ω should be set to the $\mathcal{E}(q,\omega)$ equal to zero. Since, on the other hand, $W(r)$ depends on the coordinate r, the dependence $\mathcal{E}$ on q should be kept.

In the case of a degenerate electron gas the dielectric function [2,3]

$$\mathcal{E}(q,\omega)\big|_{\substack{q\to 0\\ \omega=0}} = 1 + \frac{4\pi e^2}{Vq^2}\sum_p -\left(\frac{\partial f(p)}{\partial E(p)}\right), \tag{6}$$

can be represented as

$$\mathcal{E}(q,0) = 1 + \frac{4\pi e^2}{q^2}\frac{2}{(2\pi\hbar)^3}\int (-\frac{\partial f(p)}{\partial E(p)}) d^3 p, \tag{7}$$

where $\hbar$ is Planck's constant, and the sum over the p is replaced by the integral according to the rule

$$\frac{1}{V}\sum_p f\big(E(p)\big) \approx \frac{1}{V}\frac{V}{(2\pi\hbar)^3}\int d^3 p f\big(E(p)\big). \tag{8}$$

In the case of a degenerate electron gas, when the distribution function is represented by a step, the derivative $\left(-\frac{\partial f(p)}{\partial E(p)}\right)$ reduces with good accuracy to the δ function

$$\left(-\frac{\partial f(p)}{\partial E(p)}\right) \approx \delta(E - E_F) \ . \tag{9}$$

Substituting (9) into (7) and using the dispersion, here E_F is Fermi energy

$$E(p) = \frac{p^2}{2m_0} \quad , \tag{10}$$

and integrating with the δ–function, we obtain

$$\mathcal{E}(q,0) = 1 + \frac{4\pi e^2}{q^2} \cdot \frac{2}{(2\pi\hbar)^3} \cdot 2\pi(2m_0)^{3/2} \cdot E_F^{1/2}, \tag{11}$$

where m_0 is the electron mass.

The density of a degenerate electron gas n is related to the Fermi energy E_F by the relation [2]

$$E_F \equiv \mu(0) = (3\pi^2)^{2/3} \frac{\hbar^2}{2m_0} \cdot n^{2/3}, \tag{12}$$

where n is the electron concentration.

There fore, we can write (11) through the electron density$n$:

$$\mathcal{E}(q,0) = 1 + \frac{4\pi e^2}{q^2} \cdot \frac{n}{E_F} \cdot \frac{3}{2} = 1 + \frac{\lambda_p^2}{q^2} \quad , \tag{13}$$

where

$$\lambda_p^2 = \frac{4\pi e^2 n}{E_F} \cdot \frac{3}{2}. \tag{14}$$

For nondegenerate electron gas, the function $f(p)$is reduced to the Boltzmann distribution [2]

$$f(E) = exp\frac{\mu(T)}{T} exp\left[-\frac{E}{T}\right] = A\ exp\left[-\frac{E}{T}\right] \tag{15}$$

The derivative of the distribution function (7) in this case is equal to $\left(-\frac{\partial f(p)}{\partial E(p)}\right)$.

Substituting the derivative into $\mathcal{E}(q,0)$ from (7), we have

$$\mathcal{E}(q,0) = 1 + \frac{4\pi e^2}{q^2} \cdot \frac{2}{(2\pi\hbar)^3} \cdot \frac{1}{T} \int f(p) d^3p, \tag{16}$$

where T is the temperature.

Since the concentration of electrons can be written in the form $n = \frac{2}{(2\pi\hbar)^3} \cdot \int f(p) d^3p,$ then (16) takes the form

$$\mathcal{E}(q,0) = 1 + \frac{4\pi e^2}{q^2} \cdot \frac{n}{T} = 1 + \frac{\lambda_{np}^2}{q^2}, \tag{17}$$

where

$$\lambda_{np}^2 = 4\pi e^2 \cdot \frac{n}{T} \ . \tag{18}$$

Here Fourier component of the screened Coulomb potential is

$$U_q = \frac{W_q}{\mathcal{E}(q,\omega)} \tag{19}$$

behaves as follows

$$U_q = \frac{W_q}{\mathcal{E}(q,\omega)} = \frac{4\pi e^2}{q^2+\lambda^2} \cdot \frac{1}{V}. \tag{20}$$

In the long wavelength limit $q \to 0$, and the pole in $\mathcal{E}(q,0)$ is compensated by the pole in W_q. This leads to the disappearance of the long–range part of the initial Coulomb potential.

The inverse Fourier transform can be used to find the screened Coulomb potential $U(r)$ as

$$U(r) = \frac{e^2}{|r|} e^{-\lambda r} \tag{21}$$

From (21) it follows that at $r = 0$, this potential behaves like a Coulomb potential, and at large r it is "cut off" along the length $\sim\lambda^{-1}$. For this reason, the quantity λ^{-1} is called the screened radius $r_S = \lambda^{-1}$.

For a degenerate electron gas r_S is

$$r_{S_p}^2 = \frac{E_F}{4\pi e^2 n} \cdot \frac{2}{3}. \tag{22}$$

In a classical nondegenerate electron gas, we have

$$r_{S_{np}}^2 = \frac{T}{4\pi e^2 n}. \tag{23}$$

The change in the impurity potential due to the redistribution of the electronic charge is called electrostatic screening of the impurity potential. In both cases, the screening radius decreases with increasing electron concentration.

In metals, the electron concentration is of the order of 10^{22} cm^{-3}, and the screening radius reaches values on the order of interatomic distances.

In semiconductors, the electron concentrations vary in a wide range from 10^{16} cm^{-3} to 10^{20} cm^{-3}. Accordingly, the screening radius turns out to be larger than the crystal lattice constant.

In the classical case, the screening radius (23) was obtained in the theory of strong electrolytes by Debye and Hückel. It is often referred to as the Debye–Hückel shielding radius.

The transformation of the long–range Coulomb potential (1) into the short–range screened Coulomb potential (21) occurs due to the screening action of the electron gas with interelectronic interaction. In Fig.1. the dependence for the Coulomb and electronized Coulomb potentials is given.

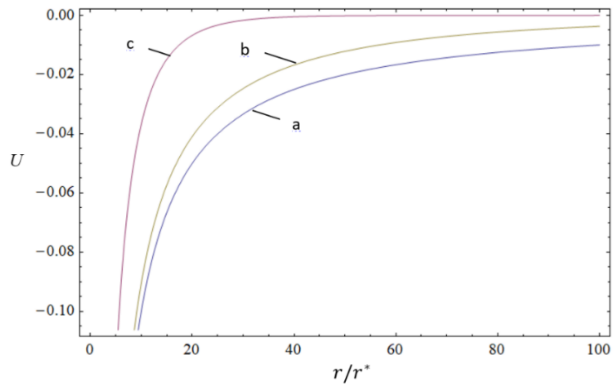

Fig. 1. Coulomb (curve *a*) and screened Coulomb (curve *b* – in case $r_S = 10r^*$ and *c* – $r_S = 100r^*$) potentials in relative terms.

A decrease in the radius of action of the screened potential compared to the Coulomb potential significantly reduces the probability of electron scattering by impurities.

Conclusions

- In this paper, the analytical matching of the changes of the screened external potential by the electron gas was considered.
- The screened Coulomb potential $U(r)$ is found using the inverse Fourier transform of the component.
- The value of the screening radius r_s for a degenerate and non–degenerate electron gas is obtained. The dependence of $r_s(\lambda^{-1})$ on potentials is presented.
- It is shown that the screening radius decreases with increasing the electron density.

Conflicts of interest

The authors declare no conflict of interest.

Author Contributions

- The author A.I. Soghomonyan raised the idea, carried out theoretical analyses, participated the writing and approval of the article;
- The authors S.A. Mkhitaryan and J.P. Markosyan participated in the theoretical analyses and in the writing and approval of the article.

Declaration of Competing Interest

The authors have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this article.

Acknowledgment

The authors would like to thank the Institute of Applied Problems of Physics at the NAS of the RA for providing all facilities to make this work complete.

References

[1] J. Ziman. Principles of the theory of solids. (M., Mir, 974). 472 p. (In Russian)
[2] Ch. Kittel. Elementary solid state physics. (M., Nauka, 1965). 366 p. (In Russian)
[3] Ch. Kittel. Introduction to solid state physics. (M., Science, 1978). 696 p. (In Russian)
[4] L.D. Landau, E.M. Lifshits. Static physics, P. 1. (M., Nauka, 1976). 264 p. (In Russian)
[5] E.M. Lifshits, L.P. Pitaevskii. Static physics, P. 2. (M., Наука, 1978). 414 p. (In Russian)