PUBLIKACIJE ELEKTROTEHNIČKOG FAKULTETA UNIVERZITETA U BEOGRADU
PUBLICATIONS DE LA FACULTÉ D'ÉLECTROTECHNIQUE DE L'UNIVERSITÉ À BELGRADE

SERIJA: MATEMATIKA I FIZIKA — SÉRIE: MATHÉMATIQUES ET PHYSIQUE

№ 274 — № 301 (1969)

299. ON THE PROBLEM OF IONISED IMPURITY SCATTERING IN SEMICONDUCTORS*

Zoran Popović

Introduction

The formula for the screening length of the scattering potential will be derived in two ways, using statistical method and quantum theory. It will be shown that the results agree with those of BROOKS and HEERING [1], [2], [3], which were published without derivation. In addition, we will discuss the problem of effective number of ionised impurities which was not considered earlier.

Statistical treatment of the problem

The potential originating from a single impurity (we assume it to be ionised) satisfies POISSON equation:

$$\Delta\varphi = -\frac{\varrho}{\varepsilon} = -\frac{e}{\varepsilon}\,(p - n + N_D^+ - N_A^-), \tag{1}$$

where concentrations p-of holes, n-of electrons, N_D^+ —of ionised donors and N_A^- —of ionised acceptor are functions of the space coordinates. As a whole, the crystal is neutral so the average value of charge density ϱ is equal to zero, supposing homogenous material, i. e.:

$$p_0 - n_0 + N_{D_0}^+ - N_{A_0}^- = 0, \tag{2}$$

where the subscript 0 denotes average value. The changers of concentrations n, p, N_D^+, N_A^- due to existence of the impurity potential are governed by BOLTZMAN and FERMY-DIRAC distributions:

$$n = n_0 \exp(e\psi/kT), \qquad p = p_0 \exp(-e\varphi/kT),$$

$$\bar{n}_D = \left(\frac{g_0}{g_1} \exp\frac{W_1 - W_f - e\psi}{kT} + 1\right)^{-1}, \quad \bar{p}_A = \left(\frac{g_0'}{g_1'} \exp\frac{W_1' - W_f' + e\varphi}{kT} + 1\right)^{-1}, \tag{3}$$

where $N_D^+ = (1 - \bar{n}_D)\, N_D$, $N_A^- = (1 - \bar{p}_A)\, N_A$; $\bar{n}_D$ and $\bar{p}_A$ are probabilities for donor and acceptor centers to be occupied with electron and hole respetively. We choose the potential φ to be zero at infinity.

---

* Presented June 5, 1969 by D. TJAPKIN.

Substituting (2) in (1) we obtain the equation for φ that is not analytically tractable. But for large distances from the impurity, as $\varphi \to 0$, we will have $|e\varphi/kT| \ll 1$ thus enabling the equation to be linearised by expanding expressions (3) in series and retaining only linear terms in $e\varphi/kT$. Hence, for φ we obtain the equation:

$$\Delta \varphi = -\frac{e^2 n'}{\varepsilon kT}\varphi, \tag{4}$$

where

$$n' = n_0 + p_0 + N_D \bar{n}_{D0}(1-\bar{n}_{D0}) + N_A \bar{p}_{A0}(1-\bar{p}_{A0}). \tag{5}$$

The central symmetrical solution of the equation (4) satisfying boundary conditions: $\varphi \to 0$ when $r \to \infty$ and $\varphi \to \pm e/4\pi\varepsilon r$ for $r \to 0$, is

$$\varphi = \pm \frac{e}{4\pi\varepsilon r} \exp(-r/r_{sc}), \qquad r_{sc} = \sqrt{\varepsilon kT/e^2 n'}, \tag{6}$$

where r_{sc} is a screening length. Substituting $p_0 = 0$, $\bar{p}_{A0} = 0$ in the expression (5) for the effective concentration n' we obtain the known BROOKS' result:

$$n' = n_0 + \left(1 + \frac{n_0 + N_A}{N_D}\right)(n_0 + N_A), \tag{7}$$

which is valied for low temperatures and n-type semiconductor.

The basic point in this derivation is that we regard ionised impurities to be able „to move" through the crystal due to repopulation of bound states. Otherwise the derivation is identical with well known DEBYE-HÜCKEL approximation.

Quantum-mechanical approach

Now we will consider not a single but all ionised impurities in the crystal and find the scattering potential. The FOURIER expansion of the energy of an electron or hole in the potential (6) is:

$$U = \pm e\varphi = \sum_{\vec{k}} \beta(\vec{k}) \exp(i\vec{k}\cdot\vec{r}), \qquad \beta(\vec{k}) = \pm \frac{e^2/\varepsilon}{k^2 + (1/r_{sc})^2}. \tag{8}$$

We will use this result later for identification of the screening length r_{sc}.

It is known that matrix elements of the perturbation, in the case of quasi-free electron, are equal to FOURIER components of the scattering potential [4]. Transition probability is proportional to the square of the matrix element modulus, and if we suppose (as is usually done) that all the impurities scatter independently, transition probability will consequently be proportional to the number of ionised impurities N_I:

$$W(\vec{k}, \vec{k}') = \frac{2\pi}{\hbar} N_I |\beta(\vec{k}-\vec{k}')|^2 \delta(E-E'). \tag{9}$$

To find FOURIER components of the perturbating potential caused by all the impurities we start with POISSON equation (1) where we substitute for the charge density (summation goes over all donor and acceptor atoms):

$$\frac{\varrho}{e}=p-n+(1-\bar{n}_D)\sum_{\vec{R}_D}\delta(\vec{r}-\vec{R}_D)-(1-p_A)\sum_{\vec{R}_A}\delta(\vec{r}-\vec{R}_A) \tag{10}$$

With this we get automatically the equation for time-average potential. For $e\varphi/kT\ll 1$ we are able to linearise it. Thus, introducing new quantities:

$$\tilde{U}=e\varphi/kT, \qquad \gamma=e^2/kT\varepsilon, \tag{11}$$

we obtain the equation:

$$\begin{aligned}-\Delta\tilde{U}/\gamma=&-(p_0+n_0)\tilde{U}+(1-\bar{n}_{D0})\sum_{\vec{R}_D}\delta(\vec{r}-\vec{R}_D)\,[1-\bar{n}_{D0}\,\tilde{U}(\vec{R}_D)]\\&-(1-\bar{p}_{A0})\sum_{\vec{R}_A}\delta(\vec{r}-\vec{R}_A)\,[1+\bar{p}_{A0}\,\tilde{U}(\vec{R}_A)]+p_0-n_0.\end{aligned} \tag{12}$$

that can be solved expanding $\tilde{U}$ in the FOURIER series:

$$\tilde{U}=\sum_{\vec{k}}\beta_1(\vec{k})\exp(i\vec{k}\cdot\vec{r}). \tag{13}$$

Substituting (13) in (12) and using the relations [5]:

$$\Big|\sum_{\vec{R}_{A,D}}\exp(i\vec{k}\cdot\vec{R}_{A,D})\Big|^2=N_{A,D},$$

$$\begin{aligned}\Big|(1-\bar{n}_{D0})\sum_{\vec{R}_D}\exp(i\vec{k}\cdot\vec{R}_D)+(1-\bar{p}_{A0})\sum_{\vec{R}_A}\exp(i\vec{k}\cdot\vec{R}_A)\Big|^2&\\=(1-\bar{n}_{D0})^2N_D+(1-\bar{p}_{A0})^2N_A,&\end{aligned} \tag{14}$$

we obtain for the square of the FOURIER component modulus and the scattering probability:

$$\begin{aligned}|\beta_1(\vec{k})|^2&=\frac{e^4}{\varepsilon^2}\,\frac{(1-\bar{n}_{D0})^2N_D+(1-\bar{p}_{A0})^2N_A}{(k^2+\gamma n')^2},\\W_1(\vec{k},\vec{k}')&=\frac{2\pi}{\hbar}\,|\beta_1(\vec{k}-\vec{k}')|^2\,\delta(E-E').\end{aligned} \tag{15}$$

Comparing the result (15) with (8) and (9) we see that the screening length is the same because $1/r_{sc}=\sqrt{\gamma n'}$. On the other hand, the probability (9) differs from (15) in the term

$$N_I=(1-\bar{n}_{D0})N_D+(1-\bar{p}_{AD})N_A.$$

which is not equal to the corresponding term in (15)

$$(1-\bar{n}_{D0})^2 N_D + (1-\bar{p}_{A0})^2 N_A.$$

As $(1-\bar{n}_{D0})$ and $(1-\bar{p}_{A0})$ are less than unity we have $W'_1 < W$, the scattering appears to be less effective when we consider all the impurities instead of simply multiplying the scattering probability for a single impurity with the number of ionised impurities. Only in the case when all impurities are ionised the two probabilities are equal.

Conclusion

Both statistical and quantum-mechanical approaches give the same result for the screening length which is identical with that given by BROOKS, [3]. The doubtful point is the effective number of ionised impurities on which the scattering takes place. The expression (15) would be definitely correct if we knew that the time-average potential is responsible for scattering. On the other hand, if we suppose that instant configuration of ionised impurities governs the scattering, the FOURIER analysis gives a result consistent with the assumption of independent scattering on impurities with the effective concentration in the screening lenght:

$$n' = n_0 + p_0.$$

It seems that from the point of view of our approach to the problem neither of the assumptions is completely valid. The real situation might be somewhere inbetween. The electron does not „feel" neither the time-average potential nor the instant potential, and probably the real situation corresponds to a certain „mixture" of these two extreme cases which is connected with the lifetime of ionised impurity and the mean free time between collisions.

Acknowledgement. The author expresses his thanks to Prof. D. TJAPKIN for stimulating discussions on the problem.

REFERENCES

[1] ZIMAN, *Electrons and Fonons*, Oxford at the Clarendon Press. 1960 (Russian translation, pp. 163, 209).

[2] H. BROOKS, *Solid State Physics*, Editors Seitz and Turnbull V4, New York 1957 (pp. 343, 344).

[3] H. BROOKS, *Adv. Electr.* 7. 85 (1955).

[4] D. TJAPKIN, *Elekronska fizika čvrstog tela*, knjiga II, Beograd, 1964.

[5] SOMERFELD, *Optics*, New York, 1954 (pp. 191).