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Ionized impurity scattering in semiconductors

R. Resta* and L. Resca*
Department of Physics, Purdue University, West Lafayette, Indiana 47907
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Dispersive valence screening, described by the Resta model, is included in the Brooks-Herring theory of carrier mobility in semiconductors. Contrary to what has been reported to date, we find the effect of such a dispersive screening to be fairly small. Physical evidence is given for such a behavior. The reasons for the disagreement with the most recent literature are discussed. Correct numerical and analytical solutions are provided.

I. INTRODUCTION

The Brooks-Herring[1] (BH) theory of ionized-impurity scattering in semiconductors has been proposed long ago, and it is still used as a basic tool for calculating collision times and carrier mobilities.[2] Within that theory, the Coulomb potential of the impurity centers is screened by free carriers, and the dielectric response of the valence electrons is simply accounted for by the static dielectric constant of the medium $\epsilon(0)$. The scattering potential assumes thus the simple screened Coulombic form[3]

$$\varphi_D(r) = \exp(-r/R_D)/\epsilon(0)r \; . \tag{1}$$

In Eq. (1), R_D is the Debye-Hückel length[4]

$$R_D = \left(\frac{\epsilon(0)K_B T}{4\pi n_i}\right)^{1/2} , \tag{2}$$

where K_B is the Boltzmann constant and n_i is the impurity concentration. The theory has been extended to quantum statistics by Dingle,[5] and the screened potential maintains there the form of Eq. (1), with a different definition of R_D (Dingle length). The carrier screening acts over a large distance scale, and R_D is typically much larger than one bond length in all physical circumstances. As an example, $R_D = 57$ Å $= 108$ a.u. in n-doped Si at room temperature for a donor concentration of 5×10^{17} cm^{-3}.

In more recent times, a considerably better understanding of valence dielectric screening in semiconductors has been reached. For the purpose of the present paper, we refer to the simple homogeneous and isotropic model semiconductor, whose dielectric response has been widely studied within Penn[6] and Resta[7] theories. These theories are quite different and somehow complementary, but end up in results which are physically very close. The main advantage of the second one is that of being conceptually simpler and completely analytical. Both theories give, as a basic feature, a valence screening which is incomplete[8] and short range. The polarization charge of the medium is confined to a distance R from the perturbation, and R is in both theories sensibly close to one bond-length in covalent solids.

Only in the very recent literature, some authors[9,10] have undertaken the task of improving the traditional BH theory, by including valence screening effects beyond those represented by the static dielectric constant. The results obtained by these authors are intriguing: the mobility has been alternatively found enhanced[9] or reduced[10] with respect to the standard BH value. In *both* cases, the effect has been claimed to be very *large*.

This "dilemma" is solved in the present paper. The proper way to account for dispersive valence screening[11] in the potential of an ionized impurity has been pointed out quite recently by one of us.[12] Following this approach, the mobility is obtained here over a wide range of temperatures and concentrations. We find that dispersive valence screening affects only very *slightly* the mobility, contrary to what has been previously reported.[9,10] Simple physical reasons for such behavior are given.

II. POTENTIAL OF AN IONIZED IMPURITY

Surprisingly enough, the dispersive screening of the dielectric medium has not been considered until very recently in the theories of carrier screening. The first attempts in this direction are due to Csavinszky.[13,14] He proposed basically two different forms for the screened potential of a point charge in a doped semiconductor at nonzero temperature. The first potential[13] (which has not the correct behavior at small r) is weaker than the traditional $\varphi_D(r)$ of Eq. (1), while the second one,[14] claimed more reliable, is stronger. These potentials have been used by the above quoted authors[9,10] in their calculation of mobilities. The main features of both potentials are clearly shown in Fig. 1, reproduced here from Ref. 12.

The same physical problem has been solved

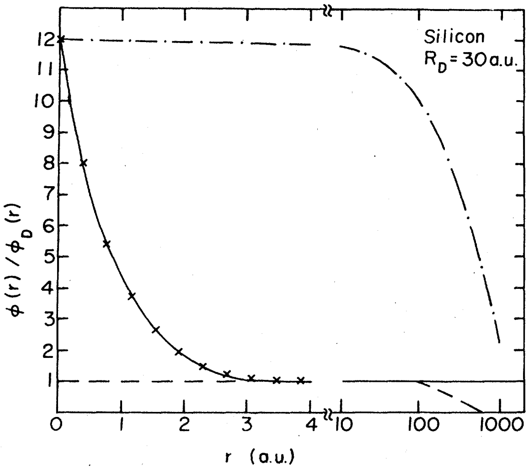

FIG. 1. Ratio of the screened potential $\varphi(r)$ to the screened Coulombic one $\varphi_D(r)$, from Eq. (1). Dashed line: Ref. 13. Dash-dotted line: Ref. 14. Crosses: numerical antitransform of Eq. (4). Solid line: approximate antitransform of Eq. (4) (for details see Ref. 12).

very recently by us in a quite recent paper,[12] hereafter referred to as I. Following a path very different from Csavinszky's one, we were able to establish a very simple and straightforward screening theory in a doped semiconductor at nonzero temperature. The main content of I can be restated in the following terms: the doped semiconductor at nonzero temperature behaves like a medium whose effective dielectric function is

$$\epsilon_{\mathrm{eff}}(k)=\epsilon(k)+\epsilon(0)R_D^{-2}k^{-2}\,, \qquad (3)$$

a result which simply amounts to sum the susceptibilities of the valence electrons and of the free carriers.[15] The approach developed in I is thus the most direct generalization of the available theories of valence screening[6,7] and carrier screening,[1,2,4,5] and it accounts correctly for the limiting behaviors of both.

When Eq. (3) is applied to the potential of a point charge, like the one of the impurity ions itself, it gives for the Fourier transform of the screened potential

$$\tilde{\varphi}(k)=4\pi/[k^2\epsilon(k)+R_D^{-2}\epsilon(0)]\,. \qquad (4)$$

The Fourier antitransform of Eq. (4) can be easily evaluated, and it is reported here in Fig. 1 for one case of interest.

Our result is the one expected on a physical ground. With reference to the distances R and R_D, as introduced in Sec. I ($R \ll R_D$), it is easily realized from Fig. 1 that carrier screening is essentially uneffective for $r<R$, and acts only for $r \simeq R_D$, while valence screening for $r>R$ enters only through $\epsilon(0)$, as in the traditional treatment.[1,2,4,5]

The same considerations can be translated in $\vec{k}$ space, a point of view of great usefulness for the following. The first term in Eq. (3) varies over a k scale of the order $1/R$,[6,7] while the second varies over $1/R_D$. This simply means that the potential $\varphi(k)$ of Eq. (4) is closely approximated at low k by $\varphi_D(k)$, the Fourier transform of Eq. (1), which can be obtained simply by replacing in Eq. (4) $\epsilon(k)$ with $\epsilon(0)$. The effect of dispersive screening[11] in Eq. (4) is therefore important only at larger k.

From Fig. 1 it is also evident that both the potentials proposed by Csavinszky are considerably different from $\varphi_D(r)$ over a large distance scale, and this of course implies that their Fourier transforms are quite apart from $\varphi_D(k)$ at low k.

Finally we must note that, after the results of I were in the process of publication, and after the present work was completed, we became aware that the approach of Csavinszky[13,14] could be corrected[16] in order to closely reproduce our previous results of I.

III. CALCULATION OF THE MOBILITY

The collision time is obtained through an angular integration[2]

$$\tau^{-1}=n_i v 2\pi\int\sigma(\theta)(1-\cos\theta)\sin\theta\, d\theta\,, \qquad (5)$$

where v is the velocity carrier and $\sigma(\theta)$ is the differential cross section for scattering from the screened impurity center. In the spirit of the BH treatment, $\sigma(\theta)$ is obtained through the first Born approximation, even though some question has been raised[17] about its applicability when the scattering potential has not the simple form of Eq. (1). The task is particularly easy here, since the screened potential has in $\vec{k}$ space the simple form of Eq. (4), and the cross section is therefore

$$\sigma(\theta)=(m^2/4\pi^2)|\tilde{\varphi}(k)|^2\,. \qquad (6)$$

In Eq. (6) m is the carrier effective mass, and

$$k=2mv\sin(\theta/2)\,. \qquad (7)$$

Inserting (6) in (5), we remain with a simple integration over $d\theta$, which can be performed numerically.

It is well known that impurity scattering in semiconductors is dominated by low-momentum transfer processes. This fact is transparent in our approach from Eqs. (4)–(6). We thus want to develop $\epsilon(k)$ in powers of k in Eq. (4) at $k=0$. We can do that very simply if we adopt Resta's analytical expression for $\epsilon(k)$ [Ref. 7(a)]. We obtain

$$\epsilon(k)\simeq\epsilon(0)(1-\alpha k^2)\,, \qquad (8)$$

TABLE I. Ratios of BH mobility over the present one for various temperatures and concentrations. The results are for silicon, with $m = 0.2987\ m_e$. The reported figures are those for which the analytical expression (13), obtained by means of the expansion (8) for $\epsilon(k)$, coincides with the numerical integration (5), obtained by means of the complete $\epsilon(k)$.

n_i (cm^{-3})	$\tau_{\mathrm{RR}}^{-1}/\tau_{\mathrm{BH}}^{-1}$ $T = 77\ ^\circ\mathrm{K}$	$\tau_{\mathrm{RR}}^{-1}/\tau_{\mathrm{BH}}^{-1}$ $T = 300\ ^\circ\mathrm{K}$
10^{15}	1.0028	1.008
10^{16}	1.0040	1.01
10^{17}	1.006	1.015
10^{18}	1.006	1.022
10^{19}	1.0020	1.03
10^{20}	1.0002	1.01
10^{21}	1.000025	1.0014

where

$$\alpha = \frac{\epsilon(0) - 1}{q^2} - \frac{R^2}{6} . \tag{9}$$

In Eq. (9), R and q are those of Ref. 7(a), and thus $\alpha = 5.54$ a.u. in silicon. Note, in this respect, the advantage of Resta's over Penn's model, *besides* the much greater analytical simplicity; at low k, Penn's model is very unreliable,[6(b),7(a)] and it would give an unphysical *positive* linear term in Eq. (8), which would largely *reverse* the correct result.

Substituting Eq. (8) in Eq. (4), the integral in Eq. (5) can be performed analytically to yield

$$\tau^{-1} = CF(v) , \tag{10a}$$

$$F(v) = \frac{-\beta^2(1 - 2A)B^{-2}}{1 + \beta^2(1 - A)} + B^{-3} \ln\left(1 + \frac{\beta^2 B}{1 + \beta^2(1 - B)/2}\right) . \tag{10b}$$

In Eqs. (10) we have defined

$$\beta = 2mvR_D , \tag{11}$$

$$A = \alpha m^2 v^2 , \tag{12a}$$

$$B = (1 + 4R_D^{-2}\alpha)^{1/2} , \tag{12b}$$

$$C = 2\pi n_i / m^3 v^3 \epsilon(0) . \tag{12c}$$

The BH result is recovered by putting $\alpha = 0$. The accuracy of Eq. (10) to reproduce Eq. (5), which fully includes Resta's $\epsilon(k)$ and we have integrated numerically, is better than 10^{-3} for any temperatures and concentrations of interest. The observations of this and of the previous paragraph are thus completely confirmed. The function $F(v)$ in Eq. (10) has exactly the same behavior as in the BH treatment.[2] Therefore, we obtain our collision time τ_{RR} from Eq. (10) as

$$\tau_{\mathrm{RR}}^{-1} = CF[(6K_B T/m)^{1/2}] . \tag{13}$$

Our mobility μ_{RR} is then related to the BH one through the equation

$$\mu_{\mathrm{RR}} = \mu_{\mathrm{BH}} \tau_{\mathrm{RR}} \tau_{\mathrm{BH}}^{-1} . \tag{14}$$

IV. DISCUSSION OF THE RESULTS

We report for convenience in Table I values of the ratio $\tau_{\mathrm{RR}}^{-1}/\tau_{\mathrm{BH}}^{-1}$ for some temperatures and concentrations. We notice that the ratio $\tau_{\mathrm{RR}}^{-1}/\tau_{\mathrm{BH}}^{-1}$ tends to unity at both high[18] and low-concentration limits at any temperature of interest. At intermediate concentrations, $\tau_{\mathrm{RR}}^{-1}/\tau_{\mathrm{BH}}^{-1}$ is greater than unity [as it has to be because of Eq. (4)] by no more than a *few* percent. The authors of Refs. 9 and 10 find alternatively very small and very large ratios for high, low, and intermediate concentrations; quite unphysical results, as stated in the conclusion of Ref. 10. This is well understandable, since if any of these calculations were correct, the BH theory could not make any sense compared to the experimental situation, which is really not the case. The reasons for such wild results are of course the inadequacies of Csavinszky potentials,[13,14] especially at large r (small k). Indeed, while our impurity potential φ is stronger than φ_D only at small r, Csavinszky's potentials[13,14] are alternatively weaker or stronger than φ_D over a wide region of space (see Fig. 1). This is unphysical and originates from an artifact in the formalism, which, however, can be corrected[16] to give results in agreement with I. In conclusion, in the present paper we have used the results of I to obtain in a simple way the analytical improvement of the BH formula for the mobility with inclusion of the valence electron dispersive screening.[19]

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*Present address: Istituto di Fisica, Università di Pisa, Italy.

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[18] In this work, we use the classical result for R_D as given in Eq. (2). For high concentrations, Fermi-Dirac statistic effects become important. To include these, values for R_D as tabulated by Dingle (Ref. 5) must be used. Note, however, that the whole BH theory becomes unreliable at high concentrations, because of the failure of several of its basic assumptions (Ref. 2).

[19] Recently, we became aware that another work on this subject was completed. It uses again the results of Ref. 13, and it suffers thus of the same drawbacks of Refs. 9 and 10. We quote it for completeness: D. E. Theodorou and H. J. Queisser, Phys. Rev. B 19, 2092 (1979).