Ionized impurity scattering in semimetals

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We developed recently a simple theory for the dielectric response of a doped semiconductor, and calculated the effect of the valence dispersive screening on the ionized-impurity-limited (IIL) mobility. The effect was found to result in a small reduction of the IIL mobility. In this paper we apply the same approach to a semimetal. In this case the effect results in a strong dielectric enhancement of the IIL mobility.

I. INTRODUCTION

The traditional theories[1-3] of ionized-impurity-limited (IIL) mobility in semiconductors describe the free carriers as moving in a background whose dielectric response is characterized by a single parameter: the static dielectric constant ϵ_0. This background is, of course, the perfect (zero-temperature, undoped) semiconductor, and the physical mechanism responsible for this static dielectric constant ϵ_0 is the polarization of valence electrons.

In two recent papers[4,5] we have provided, within the framework of the linear response theory, the generalization of these traditional theories[1-3] which includes the dispersive dielectric screening (DDS) of the background. Such a DDS has been described by means of the static dielectric function $\epsilon(k)$, calculated previously[6] within the Thomas-Fermi (TF) approximation. Since the IIL mobility is dominated by low-momentum transfer processes, it was found[5] that the inclusion of the DDS produces only a small reduction of the IIL mobility with respect to the traditional theories.[1-3]

The model semiconductor that we have considered so far is characterized by a finite value of $\epsilon(k)$ at $\vec{k}=0$, namely $\epsilon(0)=\epsilon_0$. However, it is well known that the $\epsilon(k)$ of a metal diverges as k^{-2} at low k.[7] It is thus quite natural to wonder whether materials having an intermediate behavior exist, and what would be the effect of such an intermediate DDS on the IIL mobility.

We address ourselves to these questions in this paper. Following the approach established in Refs. 4 and 5, we perform a calculation of the IIL mobility in a semimetal exhibiting a k^{-1} divergence of $\epsilon(k)$ at low k.

II. DIELECTRIC SINGULARITY OF A SEMIMETAL

The Thomas-Fermi approximation is quite effective in describing a (homogeneous and isotropic) material exhibiting either metallic or semiconducting behavior. To describe metallic behavior, the only necessary input parameter is the electronic density n_0. The semiconducting behavior is obtained by means of an alternative boundary condition (incomplete screening).[6] In this case, ϵ_0 is a second necessary input parameter. The TF theory is nonstructural and no other choices of boundary conditions are possible. Therefore, no other type of dielectric behavior can be obtained within such an approximation.

In the random-phase approximation[8] (RPA) one can consider any structural model. It is quite possible within such a theory that a particular band structure leads to some different type of dielectric behavior. For instance,

$$\epsilon(k)=\tilde{\epsilon}_0(1+\lambda k^{-1}) . \tag{1}$$

Indeed, Liu and Brust[9] have rigorously obtained within the RPA the result of Eq. (1) at low k for a band structure as in α-Sn. Later on, Liu and Tosatti[10] showed that such a dielectric singularity disappears in the doped case, as a function of k. However, a quite intimately related singularity in $\epsilon(k)$ reappears, as a function of the impurity concentration n_i.

The specific dielectric singularity given in Eq. (1) at low k arises in any perfect (zero-temperature, undoped) semiconductor in which the (completely empty) conduction band and the (completely filled) valence band touch each other at one point in $\vec{k}$ space because of symmetry.[9,10] However, we are not interested at present in studying any specific case or structural model. We can safely assume the existence of a number of materials exhibiting a dielectric behavior which is intermediate between that of a normal semiconductor and that of a metal. Our purpose is to study the implications that such a DDS would have on the IIL mobility, according to Refs. 4 and 5. We wish to study in particular the case represented in Eq. (1), since that is exactly intermediate be-

tween a metal and a normal semiconductor. We call, for convenience, such a behavior semimetallic.

III. POTENTIAL OF AN IONIZED IMPURITY

Following the approach of Refs. 4 and 5 we obtain the total static dielectric function $\epsilon_{tot}(k)$ of the doped material as

$$\epsilon_{tot}(k) = 1 + 4\pi\alpha_{tot}(k) = \epsilon(k) + (k_{TFC}/k)^2 , \tag{2}$$

where k_{TFC} is the characteristic wave vector of the free carrier polarizability. Equation (2) is obtained within the framework of the theory of the linear response in a homogeneous and isotropic medium. Equation (2) reflects the general result that the total static polarizability $\alpha_{tot}(k)$ is simply the sum of the static polarizabilities of the background and of the free carriers. Indeed, $[\epsilon(k)-1]/4\pi$ is the static polarizability of the background, whatever it is, whereas $(1/4\pi)(k_{TFC}/k)^2$ is the static polarizability of the free carriers within the TF approximation (for metallic behavior). The results of the traditional theories[1-3] are recovered by simply replacing in Eq. (2) $\epsilon(k)$ with ϵ_0.

The characteristic wave vector k_{TFC} of the free carrier polarizability is obtained within the linearized TF approximation.[11] In the completely degenerate limit it is simply related to the Fermi wave vector as[12]

$$k_{TFC}^2 = \frac{4m}{\pi} k_{FC} = \frac{4m}{\pi}(3\pi^2 n_i)^{1/3} . \tag{3}$$

In the classic limit, it is

$$k_{TFC}^2 = k_{DH}^2 = 4\pi n_i / k_B T , \tag{4}$$

where k_B is the Boltzmann constant (k_{DH}^2 is the same as in the classic Debye-Hückel theory of electrolytes except for a factor of 2). In general,

$$k_{TFC}^2 = \frac{2m^{3/2}}{\pi}(2k_B T)^{1/2} F\left(\frac{k_{FC}^2}{2mk_B T}\right) , \tag{5}$$

$$F(\eta) = \int_0^\infty \frac{\sqrt{x}\, dx}{e^{(x-\eta)}+1} . \tag{6}$$

The Fermi-Dirac integrals $F(\eta)$ were tabulated by Dingle,[3(a)] and they certainly do not represent a problem for today's computers.

We are now ready to obtain the Fourier transform of the potential of an ionized impurity (positive point charge) in the doped material. According to the linear response theory, this is simply

$$\tilde{\phi}(k) = \frac{4\pi}{k^2 \epsilon_{tot}(k)} = \frac{4\pi}{k^2 \epsilon(k) + k_{TFC}^2} . \tag{7}$$

Equation (7) reflects the general result that the dielectric screening is local and dispersive in $\vec{k}$ space (and hence translationally invariant but nonlocal in $\vec{r}$-space).[4]

In a semimetal (at low k) Eqs. (1) and (7) then yield

$$\tilde{\phi}(k) = \frac{4\pi}{\tilde{\epsilon}_0(k^2+\lambda k) + k_{TFC}^2} . \tag{8}$$

IV. IONIZED-IMPURITY-LIMITED MOBILITY

The collision time is given by the angular integration[2]

$$\tau^{-1} = n_i v 2\pi \int_0^\pi \sigma(\theta)(1-\cos\theta)\sin\theta\, d\theta , \tag{9}$$

where v is the carrier velocity and $\sigma(\theta)$ the differential cross section. Within the first Born approximation

$$\sigma(\theta) = (m^2/4\pi^2)\,|\tilde{\phi}(k)|^2 , \tag{10}$$

with

$$k = 2mv \sin(\tfrac{1}{2}\theta) . \tag{11}$$

In the completely degenerate limit, only the carriers at the Fermi surface are scattered; their velocity is

$$v = (3\pi^2 n_i)^{1/3}/m . \tag{12}$$

The IIL mobility is then given by

$$\mu = \tau/m . \tag{13}$$

It is clear from Eqs. (7)–(13) that the IIL mobility is dominated by low-k (momentum-transfer) processes. In a normal semiconductor, since $\epsilon(k) \lesssim \epsilon_0$ in that region, it has been shown[5] that the DDS of the background only produces a small reduction of the IIL mobility with respect to the traditional theories.[1-3] In Eq. (1), however, $\epsilon(k) \gg \tilde{\epsilon}_0$ at low k. In a semimetal, therefore, a strong dielectric enhancement of the IIL mobility is expected with respect to the traditional theories[1-3] ($\lambda = 0$).

The integration of Eq. (9) in a semimetal can be performed analytically. The results are reported in the Appendix. To study some examples, a numerical integration is more convenient. We do that with parameters[13] appropriate to n-doped α-Sn at 4.2 K. In that case, the carriers become completely degenerate at concentrations of the order of 10^{15} cm^{-3} or higher. We then use Eq. (3). The results are reported in Fig. 1, and compared to the result which would be given by the traditional theories[1-3] ($\lambda = 0$). We can see that there is a strong dielectric enhancement of the IIL mobility, especially at low concentrations. The effect is, however, greatly exaggerated below $n_i = 10^{15}$ cm^{-3}. In that range we should have used the general expression (5) and (6). With respect to Eq. (3), Eqs. (5) and (6) give a smaller

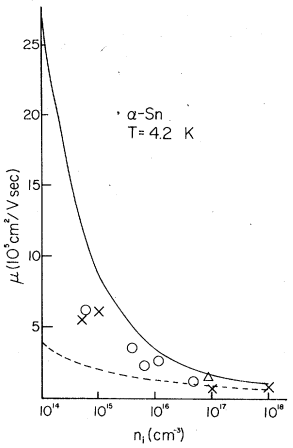

FIG. 1. IIL mobility in α-Sn at 4.2 K (Ref. 13). Form factor of Eq. (8) (solid line). Dotted line: Dingle mobility ($\lambda = 0$). Experimental data: triangle, Ref. 14; circles, Ref. 15; crosses, Ref. 16.

and smaller k_{TFC}^2, more and more as we depart from the completely degenerate limit. A smaller k_{TFC}^2 reduces the mobility, especially in the general case ($\lambda \neq 0$). In Fig. 1 we also report some experimental data,[14-16] which are consistent with the results of this approach. However, the experimental results for the IIL mobility in the specific case of α-Sn are also consistent with quite different theoretical approaches.[10,17]

In conclusion, we have shown how, in general, a dielectric singularity of the background can produce even a quite large effect on the IIL mobility of a class of materials having intermediate dielectric characteristics. Notice, in particular, that what is important for the IIL mobility is the behavior of the $\epsilon(k)$ of the background at low k, but not necessarily at $k \simeq 0$. This is expected since the factor $(1-\cos\theta)\sin\theta\, d\theta \propto k^3 dk$ strongly reduces in Eq. (9) the contribution of $|\tilde{\phi}(k)|^2$ in the immediate vicinity of the origin.

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APPENDIX

When the Dingle form factor, Eq. (8) with $\lambda = 0$, is used in Eqs. (9)–(13), one obtains[3,10,16] in the completely degenerate case[18,19]:

$$\mu_D = \tfrac{3}{2}\pi(\tilde{\epsilon}_0/m)^2[\ln(1+\beta^2) - \beta^2/(1+\beta^2)]^{-1}\,, \tag{A1}$$

where

$$\beta^2 = (2mvR_D)^2\,, \quad R_D^2 = \tilde{\epsilon}_0/k_{\mathrm{TFC}}^2\,. \tag{A2}$$

With use of the dispersive screening for semimetals at low k, Eq. (8), the mobility is

$$\mu = \frac{3}{2}\pi\left(\frac{\tilde{\epsilon}_0}{m}\right)^2\left\{\ln D + \frac{2E\beta + 2(2-F)\beta^2}{DF} - \frac{2E(2+F)}{|F|^{3/2}}\left[\mathrm{Ar}\left(\frac{E\beta+2\beta^2}{|F|^{1/2}}\right) - \mathrm{Ar}\left(\frac{E\beta}{|F|^{1/2}}\right)\right]\right\}^{-1}\,, \tag{A3}$$

$$D = 1 + \lambda R_D\beta + \beta^2\,, \tag{A4}$$

$$E = \lambda R_D\,, \tag{A5}$$

$$F = 4 - \lambda^2 R_D^2\,, \tag{A6}$$

$$\mathrm{Ar} = \text{arctanh for } F<0, \quad \mathrm{Ar} = \text{arctan for } F>0\,, \tag{A7}$$

$$\mu = \tfrac{3}{2}\pi\left(\frac{\tilde{\epsilon}_0}{m}\right)^2\left(\ln(1+\beta)^2 - \frac{3\beta+5\beta^2+4\beta^3}{(1+\beta)^3}\right)^{-1} \text{ for } F=0\,. \tag{A8}$$

Notice that Eq. (A3) reduces to (A1) for $\lambda \to 0$.

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[1]H. Brooks, Phys. Rev. 83, 879 (1951); C. Herring (unpublished).
[2]H. Brooks, *Advances in Electronics and Electron Physics*, edited by L. Marton (Academic, New York, 1955), Vol. 7, p. 85; K. Seeger, *Semiconductor Physics* (Springer, Vienna, 1973), Chap. 6
[3](a) R. B. Dingle, Philos. Mag. 46, 831 (1955); (b) R. Mansfield, Proc. Phys. Soc., London, Sect. B 69, 76 (1956).
[4]R. Resta, Phys. Rev. B 19, 3022 (1979).
[5]R. Resta and L. Resca, Phys. Rev. B 20, 3254 (1979).
[6]R. Resta, Phys. Rev. B 16, 2717 (1977).

[7]See, for instance, L. Hedin and S. Lundqvist, Solid State Phys. 23, 1 (1969).

[8]P. Nozières and D. Pines, Nuovo Cimento 9, 470 (1958); Phys. Rev. 109, 762 (1958); H. Ehrenreich and M. H. Cohen, Phys. Rev. 115, 786 (1959).

[9](a) L. Liu and D. Brust, Phys. Rev. Lett. 20, 651 (1968); (b) L. Liu and D. Brust, Phys. Rev. 173, 777 (1968). In Eq. (1) $\tilde{\epsilon}_0$ and λ are intended as parameters, with no particular physical meaning attached to them. Liu and Brust attempt a direct calculation of them in α-Sn, which, however, does not lead to meaningful results.

[10]L. Liu and E. Tosatti, Phys. Rev. Lett. 23, 772 (1969); L. Liu and E. Tosatti, Phys. Rev. B 2, 1926 (1970).

[11]See, for instance, N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, New York, 1976), pp. 341–343.

[12]Atomic units are used throughout this paper ($\hbar = e = m_e = 1$). For the sake of clarity we adopt the subscript c when we refer to free carriers, and no particular subscript when we refer to valence electrons. Notice that the TF theory for valence electrons in metals or semiconductors (Ref. 6) always refers to the free electron mass m_e, whereas for free carriers the effective mass m is used instead. This result may be better understood in the RPA limit of low k (Ref. 11). Since $k_{FC} \ll k_F$, only the bottom of the conduction band is important for free carriers, whereas the whole band is important for valence electrons.

[13]$\tilde{\epsilon}_0 = 24$, $\lambda = 3.49 \times 10^{-3}$, $m = 0.024$. See the appropriate references as quoted in Ref. 9(b).

[14]O. N. Tufte and A. W. Ewald, Phys. Rev. 122, 1431 (1961).

[15]E. D. Hinkley and A. W. Ewald, Phys. Rev. 134, A1261 (1964).

[16]C. F. Lavine and A. W. Ewald, J. Phys. Chem. Solids 32, 1121 (1979).

[17]J. G. Broerman, Phys. Rev. 183, 754 (1969); J. G. Broerman, Phys. Rev. B 1, 4568 (1970); J. G. Broerman, J. Phys. Chem. Solids 32, 1263 (1971); J. G. Broerman, L. Liu, and K. N. Pathak, Phys. Rev. B 4, 664 (1971).

[18]The collision time has the same expression as that of Brooks-Herring,[1,2] with suitable changes in k_{TFC} and v [Eqs. (3) and (12)].

[19]There is a misprint in Ref. 11. Equation (12c) should read

$$C = 2\pi n_i / m^2 v^3 \epsilon^2(0) .$$