PHYSICAL REVIEW B VOLUME 19, NUMBER 6 15 MARCH 1979

Dielectric behavior of a doped semiconductor

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(Received 17 August 1978)

The static dielectric response of a doped semiconductor at nonzero temperature is studied here in the simple homogeneous and isotropic model. The present approach generalizes the model dielectric responses proposed by Penn and by the author accounting for free-carrier screening, or equivalently it generalizes the Dingle model of carrier screening accounting for the microscopic dielectric behavior of the medium. The effect of the present model response in the screening of a point-charge potential is explicitly shown and discussed against quite different solutions recently proposed for this same physical problem.

I. INTRODUCTION

The physical problem which is discussed here is the dielectric response of a doped semiconductor at nonzero temperature to an external static disturbance.

The dielectric behavior of a covalent undoped semiconductor at zero temperature is at present well understood. Simple model dielectric functions are available,[1,2] all of which are obtained for the isotropic and homogeneous solid. It turns out that such a simple model is able to reproduce remarkably well the results of more realistic approaches.[3] The kind of charge responsible for this zero-temperature dielectric screening is mainly the charge of the valence electrons involved in crystal bonds.

On the other hand, in a doped semiconductor at nonzero temperature, beside the above charge, a different kind of charge contributes to the screening of an external field: the charge of the free carriers, either electrons in the conduction band or holes in the valence band. Under suitable conditions, not to be discussed here, the carriers behave as free particles whose mass is different from the electron mass.[4] The dielectric screening due to the free carriers has been studied long ago by Dingle,[5] under the hypothesis that the contribution of the valence electrons could be simply schematized with the static dielectric constant $\epsilon(0)$ of the pure semiconductor. If the external disturbance is a static point charge, one finds within the Dingle theory a field which is exponentially screened in a typical length R_D depending on the impurity concentration, on the temperature, and on the carrier-effective mass.

The purpose of the present paper is to develop a theory which includes on the same grounds the dielectric response of the valence electrons and that of the free carriers. The model dielectric response which is presented here can thus be seen as the generalization to the doped case of the homogeneous and isotropic model semiconductor[1,2]; or alternatively it can be seen as the generalization of the Dingle theory[5] to a medium having a k-dependent dielectric function $\epsilon(k)$.

In Sec. II the dielectric behavior of the valence charge is studied and a generalized Poisson equation is derived. In Sec. III it is shown how to account for the free carriers in screening, and an explicit form for the dielectric response is given. In Sec. IV the screened potential of a point charge is explicitly shown. In Sec. V a very recent different approach to this same physical problem is discussed.

II. MICROSCOPIC POISSON EQUATION IN A DIELECTRIC AT ZERO TEMPERATURE

The basic quantities for the description of the response of an insulator are the external field $\vec{D}$, generated by the external charge, and the screened field $\vec{E}$, generated by both the external and polarization charges. Their relationship is written

$$\vec{E} = \epsilon^{-1}\vec{D} . \tag{1}$$

For an isotropic medium, and over a macroscopic distance scale, ϵ^{-1} is a constant equal to the inverse static dielectric constant $1/\epsilon(0)$. More generally, Eq. (1) should be interpreted as an operator relationship[2,6] involving the linear response ϵ^{-1}:

$$\vec{E}(\vec{r}) = \int d\vec{r}'\, \epsilon^{-1}(\vec{r},\vec{r}')\vec{D}(\vec{r}') . \tag{2}$$

If one assumes to be dealing with an isotropic and homogeneous system, Eq. (2) becomes

$$\vec{E}(\vec{r}) = \int d\vec{r}'\, \epsilon^{-1}(|\vec{r}-\vec{r}'|)\vec{D}(\vec{r}') . \tag{3}$$

When Eq. (3) is Fourier transformed to $\vec{k}$ space, the convolution product becomes an algebraic one, and we obtain

$$\vec{E}(\vec{k}) = \vec{D}(\vec{k})/\epsilon(k) , \tag{4}$$

which generalizes straightforwardly the macro-

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scopic Eq. (1). The function $\epsilon(k)$ for a homogeneous and isotropic model semiconductor has been the object of considerable work.[1,2] As a general feature, $\epsilon(k)$ is greater than 1 and finite for any k.

In a covalent semiconductor at zero temperature, the polarization charge physically responsible for the screening mechanism is mainly due to valence electrons. They are not completely free to move, and prescriptions have been given to account for their limited polarizability, either in $\vec{k}$ space, as in the Penn model,[1] or in $\vec{r}$ space, as in the Resta model.[2] The behavior of the valence electrons here is supposed to be fully accounted for by the dielectric response. Now suppose that some external charge is introduced in the dielectric. Starting with the Maxwell equation

$$\vec{\nabla}\cdot\vec{D}=4\pi\rho_{\text{ext}}\ , \tag{5}$$

the potential φ of the screened field $\vec{E}$ can easily be shown to obey the generalized Poisson equation

$$\nabla^2\varphi(r)=-4\pi\int d\vec{r}'\,\epsilon^{-1}(|\vec{r}-\vec{r}'|)\rho_{\text{ext}}(\vec{r}')\ . \tag{6}$$

So the microscopic Poisson equation in a model dielectric is an integro-differential one. One recovers the macroscopic limit with the obvious identification

$$\epsilon^{-1}(|\vec{r}-\vec{r}'|)\to\delta(\vec{r}-\vec{r}')/\epsilon(0)\ . \tag{7}$$

In the literature on the subject,[1,2] a dielectric function of a different kind is often dubbed "spatial dielectric function" and is indicated by $\tilde{\epsilon}(r)$. This has become customary, but is somewhat misleading. It is important to stress here that $\epsilon^{-1}(r)\neq 1/\tilde{\epsilon}(r)$. The function $\tilde{\epsilon}(r)$ is useful *only* for point-charge disturbances, and operates locally on the unscreened potential,[1,2] while the linear response $\epsilon^{-1}(r)$ is a much more fundamental quantity, and operates through a convolution product[2,6] on *any* unscreened potential or field, as in Eq. (3).

The linear response $\epsilon^{-1}(r)$ is not displayed in the original literature on the isotropic and homogeneous model semiconductor.[1,2] Within the model of Ref. 2, $\epsilon^{-1}(r)$ has a very simple explicit form, which is reported here in Appendix A.

III. DIELECTRIC RESPONSE OF A DOPED SEMICONDUCTOR AT NONZERO TEMPERATURE

In a doped semiconductor at nonzero temperature, free carriers are present, and in fact the macroscopical behavior at a given temperature is the one of a conductor. Beside the valence charge, already accounted for by the zero-temperature microscopic $\epsilon(k)$, one has inside the solid two other kinds of charges: static impurity ions and free carriers. It is important to point out that the carriers can also be considered "external" in the sense of Sec. II, since their motion is quasiclassical and their interaction is instantaneously screened by the valence electrons through the dielectric function $\epsilon(k)$.[4] We call the impurity-ion charge density $\rho_i(\vec{r})$ and the carrier density $\rho_c(\vec{r})$. Finally, suppose that this doped semiconductor is perturbed by an external charge (a really external one, this time!) which we call $\rho_{\text{free}}(\vec{r})$. So the kind of charges to be considered "external" in the sense of Sec. II and to be inserted in Eq. (6) are in all three:

$$\rho_{\text{ext}}(\vec{r})=\rho_c(\vec{r})+\rho_i(\vec{r})+\rho_{\text{free}}(\vec{r})\ , \tag{8}$$

although ρ_c and ρ_i actually belong to the doped semiconductor.

Now $\rho_{\text{free}}(\vec{r})$ is supposed to be given; $\rho_i(\vec{r})$ too, being the fixed impurity ions. The real problem is to find $\rho_c(\vec{r})$. The carriers are completely free to move, and a relationship between their density $\rho_c(\vec{r})$ at a given temperature and the electrostatic potential is provided by statistical mechanics. This point has been worked out by Dingle,[5] starting from the Fermi-Dirac distribution function and making some suitable approximations. His basic result, from the point of view of the present paper, can be restated as the assumption of a linear relationship of the kind (in atomic units $\hbar=1$, $m_e=1$, $e^2=1$):

$$\rho_i(\vec{r})+\rho_c(\vec{r})=-[\epsilon(0)/4\pi R_D^2]\varphi(\vec{r})\ , \tag{9}$$

where R_D is known as the Dingle screening length,[5] and can be calculated with the use of Fermi-Dirac integrals as a function of the carrier-effective mass m_*, the temperature T, and the impurity density n_i. In the classical Boltzmann limit the Dingle length goes to

$$R_D^2\to\epsilon(0)\kappa T/4\pi n_i\ , \tag{10}$$

where κ is the Boltzmann constant. Note that it becomes independent of the effective mass. A typical value for R_D at room temperature in n-doped silicon at a donor concentration of 5×10^{17} cm^{-3} is $R_D\approx 60$.

Now we are ready to substitute (9) in (8), and (8) in the integro-differential equation (6) to obtain the generalized Dingle equation

$$\nabla^2\varphi(r)-R_D^{-2}\epsilon(0)\int d\vec{r}'\,\epsilon^{-1}(|\vec{r}-\vec{r}'|)\varphi(\vec{r}')=-4\pi\int d\vec{r}'\,\epsilon^{-1}(|\vec{r}-\vec{r}'|)\rho_{\text{free}}(\vec{r}')\ . \tag{11}$$

The meaning of this equation is more transparent in $\vec{k}$ space, since it becomes

$$[k^2+R_D^{-2}\epsilon(0)/\epsilon(k)]\varphi(\vec{k})=4\pi\rho_{\text{free}}(\vec{k})/\epsilon(k)\ . \tag{12}$$

This means that the doped semiconductor at nonzero temperature responds to a static perturbation as a medium whose effective dielectric function is

$$\epsilon_{eff}(k) = \epsilon(k) + \epsilon(0) R_D^{-2} k^{-2} . \quad (13)$$

For large k, $\epsilon_{eff}(k) \approx 1$, and this means that perturbations rapidly varying in $\vec{r}$ space are essentially unscreened. On the other hand for small k, $\epsilon_{eff}(k)$ diverges like k^{-2}, as expected in a conductor. Moreover, this divergence has a coefficient which is proportional, at least in the classical limit of Eq. (10), to the impurity concentration and to the inverse temperature. What a nice result.

IV. GENERALIZED DINGLE POTENTIAL

Suppose now that ρ_{free} is simply a point charge

$$\rho_{free}(\vec{r}) = Q\delta(\vec{r}) . \quad (14)$$

The solution of (11) with the correct boundary conditions is easily found in $\vec{k}$ space from (12)

$$\varphi(k) = 4\pi Q / [k^2 \epsilon(k) + R_D^{-2} \epsilon(0)] . \quad (15)$$

Given a model $\epsilon(k)$, the antitransform of (15) yields straightforwardly the generalized Dingle potential. The standard Dingle treatment is exactly recovered in any of the preceding Eqs. (11)–(15), when the substitution (7) is made, or equivalently $\epsilon(k) \to \epsilon(0)$. So the standard Dingle potential[5] is, from (15)

$$\varphi_D(r) = Q \exp(-r/R_D)/\epsilon(0) r . \quad (16)$$

On the other hand, the usual screened potential for the undoped semiconductor is obtained from Eq. (15) by simply taking the $R_D \to \infty$ limit. If use is made of the "spatial dielectric function" $\bar{\epsilon}(r)$, defined as is customary in the literature,[1,2] the Fourier transform of Eq. (15) is written

$$\varphi(r) = Q/\bar{\epsilon}(r) r, \quad R_D \to \infty . \quad (17)$$

The present generalization, Eq. (15), can be used to demonstrate the two limiting cases discussed above for $k \to 0$ and $k \to \infty$. Therefore the antitransform of Eq. (15) is expected to behave like Eq. (16) for large r and like Eq. (17) for small r. Moreover, since the typical r over which $\bar{\epsilon}(r)$ varies[1,2] is much smaller than any physical value of R_D, a reasonable guess for the antitransform of Eq. (15) is

$$\varphi(r) \approx Q \exp(-r/R_D)/\bar{\epsilon}(r) r . \quad (18)$$

The numerical antitransform of Eq. (15) in silicon has been performed for $R_D = 30$ and $R_D = 60$, with $\epsilon(k)$ taken from Ref. 2. Technical details about this antitransform are given in Appendix B. The results turned out to be extremely close to the approximate analytical expression (18). The ratio $\varphi(r)/\varphi_D(r)$ obtained in silicon for $R_D = 30$ is displayed in Fig. 1. Its approximated analytical form is, from Eq. (18),

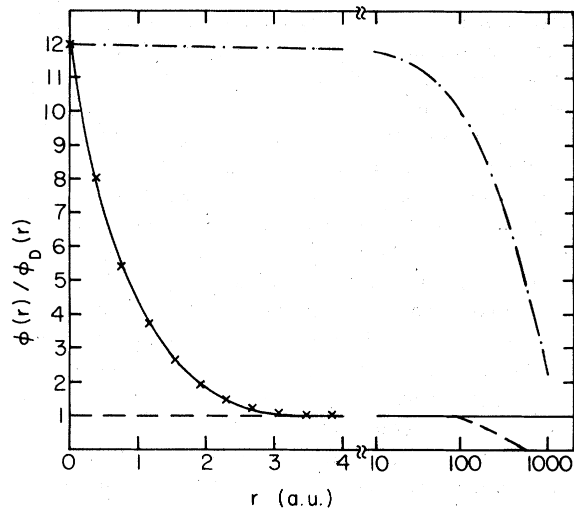

FIG. 1. Ratio of the generalized Dingle potential to the standard Dingle potential in silicon for $R_D = 30$. Crosses: numerical antitransform; solid line: Eq. (19); dashed line: Ref. 7; dash-dotted line: Ref. 8.

$$\varphi(r)/\varphi_D(r) \approx \epsilon(0)/\bar{\epsilon}(r) ; \quad (19)$$

as is easily seen, it is exactly coincident with the numerical result in the drawing's scale. The two other curves shown in Fig. 1 are discussed in Sec. V.

Results of the kinds obtained in Eqs. (18) and (19) were expected on physical grounds: in fact the carrier screening acts over a much larger distance scale than the valence screening; therefore for short distances one has essentially the potential of the undoped semiconductor, while for distances larger than the single-bond length one has the Dingle potential.

V. RELATIONSHIP WITH DIFFERENT THEORIES

The same physical problem discussed in Sec. IV has been recently tackled by Csavinszky in a series of papers[7–10] based on a completely different formalism. In his first paper he proposed[7] a potential $\varphi(r)$ which has not the correct behavior at small r (dashed line in Fig. 1). This is acknowledged in Ref. 8, where the way to overcome this drawback is outlined and an approximate $\varphi(r)$ having the correct limiting behavior is explicitly given (dash-dotted line in Fig. 1). In this last case,[8] the analytical form of $\varphi(r)$ proposed by Csavinszky turns out to be identical to Eq. (18); but the exponential function has a decay length which is quite different from R_D and the whole result is physically very far from the one found here (see Fig. 1).

The reasons for the disagreement are pretty clear. Starting from the macroscopic Eq. (1),

Csavinszky proceeds by assuming an algebraic product of spatial functions [see Eq. (A2) of Ref. 7] and uses the dielectric function $\bar{\epsilon}(r)$. The generalization of Eq. (1) proposed here on the grounds of linear response theory is completely different, as discussed in detail in Sec. II. As a matter of fact, the whole conception of a Penn-model semiconductor as a "medium with spatially variable dielectric constant"[7-10] is misleading, for the linear case at least. Going just beyond the linear response theory, as has been recently done by some authors,[10,11] the concept of "spatially variable dielectric constant" could perhaps be useful. Within the linear theory, a homogeneous and isotropic model semiconductor[1,2] is actually a medium with a k-dependent dielectric constant, and this means that the response of the valence electrons to an external perturbation is nonlocal in $\vec{r}$ space, as in Eqs. (2), (3), and (6).

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation Grant No. DMR76-04775 and NSF/MRL Program No. DMR76-00889, and by Consiglio Nazionale delle Richerche through its GNSM unit in Pisa. The author is grateful to Dr. L. Resca for stimulating and useful discussions. He is also indebted to the Physics Department of Purdue University for its hospitality while this work was being done.

APPENDIX A: EXPLICIT EXPRESSION FOR $\epsilon^{-1}(r)$

An explicit expression for the linear response $\epsilon^{-1}(r)$ of a homogeneous and isotropic model semiconductor can be obtained very simply in the framework of Ref. 2. This paper (and its equations) will be referred to as I in the following.

The main quantities of the theory are the inverse Thomas-Fermi screening length q and the screening radius R, which is found as the root of

$$\sinh qR/qR = \epsilon(0). \tag{A1}$$

An explicit expression for $\epsilon(k)$ is given in Eq. (I-21). The Fourier antitransform of $1/\epsilon(k)$ can be performed analytically to obtain $\epsilon^{-1}(r)$. This is straightforward, but tedious. Better insight is obtained in deriving the same result through the generalized Poisson equation introduced here as Eq. (6). Suppose ρ_{ext} is simply a point charge

$$\rho_{ext}(\vec{r}) = \delta(\vec{r}); \tag{A2}$$

then Eq. (6) becomes

$$\epsilon^{-1}(r) = -\nabla^2\varphi(r)/4\pi. \tag{A3}$$

The screened potential of a point charge is explicitly found in I. From Eq. (I-14) one has

$$\nabla^2\varphi(r) = 0, \quad r \geq R. \tag{A4}$$

Combining Eqs. (I-9) and (I-10):

$$\nabla^2\varphi(r) = -4\pi\delta(\vec{r}) + q^2[\varphi(r) - A], \quad r \leq R. \tag{A5}$$

Using in (A5) the explicit expression for $\varphi(r) - A$, Eqs. (I-13) and (I-16), the final result can be recast in the form

$$\epsilon^{-1}(r) = \delta(\vec{r}) - \frac{q}{4\pi\epsilon(0)R}\frac{\sinh q(R-r)}{r}\theta(R-r), \tag{A6}$$

where θ is the Heaviside distribution.

It is interesting to recover the macroscopic limit, Eq. (7), from Eq. (A6). The typical lengths appearing in Eq. (A6) are R and $1/q$. Over a scale of distances large with respect to both R and $1/q$, $\epsilon^{-1}(r)$ behaves like

$$\lim_{R\to 0, q\to\infty} \epsilon^{-1}(r) = \delta(\vec{r})/\epsilon(0). \tag{A7}$$

The proof of (A7) is straightforward, once paid attention to the fact that in this limitng process the product qR must be kept constant, in order to conserve Eq. (A1).

APPENDIX B: NUMERICAL ANTITRANSFORM OF THE SCREENED POTENTIAL

The Fourier antitransform of Eq. (15) is

$$\varphi(r) = \frac{2Q}{\pi r}\int_0^\infty \frac{k \sin kr\, dk}{\epsilon(k)k^2 + \epsilon(0)R_D^{-2}}. \tag{B1}$$

Put in this form, it is not suitable for numerical treatment since the integral is not absolutely convergent. Convergence is improved with a simple trick. Consider the expression

$$\psi(r) = \frac{2Q}{\pi r}\int_0^\infty \left(\frac{1}{\epsilon(k)k^2 + \epsilon(0)R_D^{-2}} - \frac{1}{k^2 + \epsilon(0)R_D^{-2}}\right) k \sin kr\, dk, \tag{B2}$$

where the difference between $\psi(r)$ and $\varphi(r)$ is an integral which is easily performed analytically. Now the integral in (B2) can be evaluated numerically, being its convergence much faster. When $\epsilon(k)$ is taken from Ref. 2, the integrand in (B2) is of the order of k^{-3} for large k.

The numerical evaluation of $\psi(r)$ has been performed with the use of a standard fast-Fourier-transform routine,[12] and $\varphi(r)$ has been reconstructed simply by addition of the analytical dif-

ference. Excellent convergence has been reached for either $R_D = 30$ or $R_D = 60$ using 2^{14} points and a k step of 0.001. As a result, one obtains a tabulation with an r step of 0.38 in an execution time of 17 seconds on a CDC 6500-1 computer. The ratio $\varphi(r)/\varphi_D(r)$ obtained is quite good until the absolute value of $\varphi(r)$ becomes $\approx 10^{-4}$, that is up to $r \approx 200$ for $R_D = 30$ and $r \approx 400$ for $R_D = 60$.

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