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Nonlinear impurity screening in semiconductors

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Nonlinear impurity screening in metals has been widely studied in the literature, and the differences with respect to the linear results have been found to be important. The screening theories available for semiconductors were until very recently obtained in $\vec{k}$ space, and this prevented the study of nonlinear effects. We present here for the first time an investigation of nonlinear impurity screening in a model semiconductor. The Thomas-Fermi theory of dielectric screening, recently developed by one of us, has been used. Nonlinearity effects are found to be of the same order of magnitude as in metals. A remarkable donor-acceptor asymmetry is also found.

I. INTRODUCTION

The field of an ionized impurity in a semiconductor is a subject of relevant interest, which has been widely discussed in the literature.[1] The bare impurity potential must be screened to account for the dielectric relaxation of the host, and this has always been done, according to the authors' best knowledge, within the linear-response theory.[1-6] Linearization is exact, in principle, for vanishingly small impurity charges,[2] but the question arises whether the approximation is good for integer values of the charge Z (in a.u.). In the case of metallic screening, the effects due to nonlinear relaxation have been investigated by many authors and found to be important.[7-10]

Throughout this paper we adopt the homogeneous and isotropic model solid (HIMS) hypothesis, which has been adopted in the literature for the study of nonlinear response in metals.[8-10] Despite the anisotropy and inhomogeneousness of covalent bonding, the HIMS has proved to be a very good approximation for the linear response of a real semiconductor,[5,6] and a very useful tool for the interpretation of a number of physical properties.[11]

In this paper we study the nonlinear response of a model semiconductor to a static-point-charge external disturbance, whose bare (unscreened) potential is

$$V_0(r) = -Z/r\,. \tag{1}$$

Until very recently all the approaches to the problem of dielectric screening in a semiconductor were made in $\vec{k}$ space,[1,5,6] starting from the random-phase-approximation (RPA) formalism.[3] The intrinsic linearity of the Fourier transform obviously prevents the possibility of dealing with any nonlinear effect. In $\vec{r}$ space, on the other hand, wave-function approaches have been used within the cluster approximation for the study of deep-lying impurity states.[12] Any wave-function method, however, seems to be inadequate for the field of a shallow impurity, since the number of electrons involved in semiconductor screening is typically noninteger. If $\epsilon(0)$ is the static dielectric constant of the semiconductor, the screening charge is, in fact, $Z[1-1/\epsilon(0)]$.

For metals, linear and nonlinear impurity screening was widely investigated long ago within the Thomas-Fermi (TF) model.[7,8] Recent work has shown the correctness of the TF results.[9,10] The statistical TF method is an $\vec{r}$-space approach which avoids the use of a wave function, thus allowing the handling of a noninteger number of electrons. Only very recently this possibility was fully exploited in a paper by one of us,[13] hereafter referred to as I. In that paper the general theory of TF screening in semiconductors was developed and the linearized TF screening equation was explicitly solved in a closed analytical form. The TF linear-response functions were found to be in excellent agreement with the same functions evaluated in the literature within $\vec{k}$-space theory.[5,6] The TF approach yields naturally the way to study nonlinearity, since the main equation comes out nonlinear and is then linearized.

We present in this paper the numerical solution of the nonlinear TF equation for point-charge screening, for different values of the impurity charge Z. We found important deviations from the linear results, and a strong donor-acceptor asymmetry. The nonlinear screening of an impurity pseudopotential different from (1) is also briefly discussed.

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II. THEORY AND COMPUTATION

We refer to Paper I for the derivation of the Mott equation[7] for TF point-charge screening, as well as for the discussion of the semiconductor boundary conditions. We use atomic units: $e^2=1$, $\hbar=1$, $m_e=1$. The displaced charge density in a semiconductor has finite radius R, and the equations to be solved for the self-consistent screened potential $V(r)$ are

$$\nabla^2 V(r) = (2^{7/2}/3\pi)\{E_F^{3/2} - [E_F + V(R) - V(r)]^{3/2}\}, \quad r \leq R\,; \tag{2}$$

$$\nabla^2 V(r) = 0\,, \quad r \geq R\,, \tag{3}$$

where E_F is the valence Fermi energy.

An additional complication arises for negative Z (see Fig. 1 of Paper I), since in the neighborhood of a repulsive impurity a Coulomb hole is originated, inside which the electron density is zero. The same problem for metals has been discussed by Alfred and March.[14] If the radius of the Coulomb hole is R_C, Eq. (2) is valid only for $r \geq R_C$, while for $r \leq R_C$ the equation is

$$\nabla^2 V(r) = (2^{7/2}/3\pi)E_F^{3/2}, \quad r \leq R_C\,, \tag{4}$$

because only the uniform background is present, with no electron, consistent with the HIMS hypothesis.

The acceptable solution of (3) n a semiconductor whose static dielectric constant is $\epsilon(0)$ is

$$V(r) = -Z/\epsilon(0)r\,, \quad r \geq R\,. \tag{5}$$

For a given R, Eq. (2) can be numerically solved backwards, matching the potential and its first derivative at R with (5). R is then varied until the solution has the correct behavior at the origin. For positive Z this means for the solution of (2) the condition

$$\lim_{r\to 0} rV(r) = -Z\,. \tag{6}$$

For negative Z, the procedure is only slightly more complicated. The range of validity of (2) is further limited by

$$V(r) \leq -Z/\epsilon(0)R + E_F\,, \tag{7}$$

where the equal sign holds for $r=R_C$, the Coulomb hole radius. Inside this radius the general solution of (4), with the correct behavior (6) at the origin, is

$$V(r) = -Z/r + (2^{5/2}/9\pi)E_F^{3/2}r^2 + \beta\,, \quad r \leq R_C\,. \tag{8}$$

β is easily found by imposing the continuity of $V(r)$ at $r=R_C$. Then the matching of the derivative of $V(r)$ at R_C is obtained, iterating the whole procedure for different values of the starting screening radius R.

In numerical work, the initial-value problem for Eq. (2) was solved with the use of Hamming's modified predictor-corrector method,[15] and the final matching of functions was always obtained within 10^{-3}.

III. RESULTS FOR DIAMOND, SILICON, AND GERMANIUM

The valence Fermi energies used in Paper I were all relative to four valence electrons per atom. Actually the filled $3d$ orbitals of Ge are partially involved in the valence charge density. According to the Phillips–Van Vechten theory of ionicity an effective number of valence electrons per atom can be defined in a wide class of solids.[11] In the present paper we use the Fermi energies corresponding to these effective numbers, which turn out to be 4, 4, and 5, respectively in diamond, Si, and Ge.

It should be noted that the linear-screening radii R evaluated in Paper I were slightly smaller than the single bond length in diamond and Si, while the opposite happened for Ge (see Table I of Paper I). With the above assumptions about the valence-electron density Ge is no longer anomalous, but on the contrary it follows the general trend.

The nonlinear problem discussed in Sec. II has been solved in diamond, Si, and Ge for $Z=\pm 1, \pm 4$. The screening radii R and the Coulomb radii R_C are shown in Table I. In order to display the screened potential $V(r)$, it is convenient to introduce an effective spatial dielectric function $\bar{\epsilon}(r)$, defined simply by

$$V(r) = -Z/\bar{\epsilon}(r)r\,. \tag{9}$$

The $\bar{\epsilon}(r)$ resulting from the present calculation are shown in Figs. 1–3. It is easily seen that nonlinear effects tend to make the screening more effective for attractive potentials, while the opposite happens for repulsive ones.

The deviations from linear behavior appear to be of the same order of magnitude as those found for

TABLE I. Relevant figures for nonlinear screening. The linear results have been labeled as $Z=0$. For the difference from Ref. 13 in Ge see text.

	Z	Diamond	Silicon	Germanium
Screening radius R (a.u.)	4	2.44	3.74	4.02
	1	2.64	4.06	4.33
	0	2.76	4.28	4.54
	−1	2.93	4.63	4.86
	−4	3.30	5.28	5.47
Coulomb hole radius R_C	−1	0.53	0.97	0.93
	−4	1.21	2.06	1.98

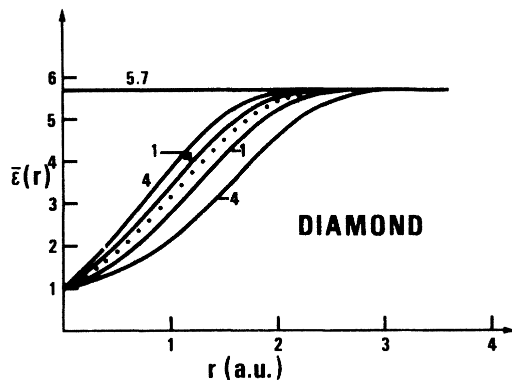

FIG. 1. Effective spatial dielectric constant for diamond. The dotted line is the linear result, from Paper I.

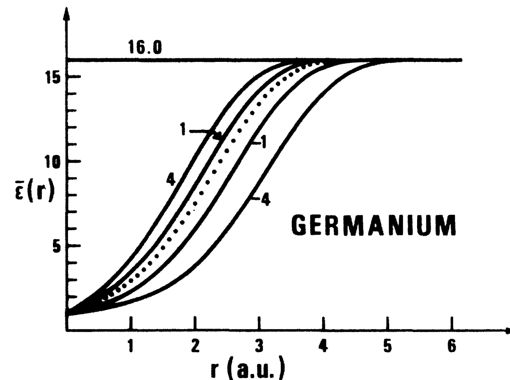

FIG. 3. Effective spatial dielectric constant for Ge. The dotted line is the linear result. The Fermi energy has been changed from Paper I, see text.

metals in the literature.[8-10] A strong asymmetry occurs when the sign of Z is reversed. This donor-acceptor asymmetry cannot be found in the linear context, and should be accounted for in the calculation of the impurity levels.

IV. SOME FURTHER CONSIDERATIONS

A. Charge densities and pair correlation

The charge distribution around a monovalent repulsive impurity has been sometimes compared to the pair-correlation function.[9] The two quantities have a different theoretical meaning, since the former is purely static effect, while the latter includes dynamical information. Nonetheless, these two quantities have been found to be close enough in metals,[9] and this fact has the appealing meaning that the correlation hole around a given electron of the solid resembles the charge distribution around a static negative point charge.

In Fig. 4 we show the charge distribution around a $Z=-1$ point charge in Si, as given from the present TF calculation, and divided by n_0. It is zero for $r \leq R_C$, then it increases and it reaches 1 at $r=R$. For a comparison the pair-correlation function of an electron gas at the same density is also shown in two different approximations. One is the well known RPA pair-correlation function,[16] which has the serious drawback of becoming negative at short r. The second one is the most accurate available pair-correlation function, calculated by Singwi *et al.*[17]

It should be noted that the total charge of the correlation hole is 1, according to the number sum rule for the electron gas,[18] while the static-induced charge in a semiconductor is $1-1/\epsilon(0)$, as pointed out in Sec. I.

B. Pseudopotential screening

The bare impurity potential considered so far in the present paper was the pure Coulomb one, Eq. (1). In more refined impurity calculations[1] a pseudopotential approach is adopted, where the Coulomb potential (1) is modified by a short-range

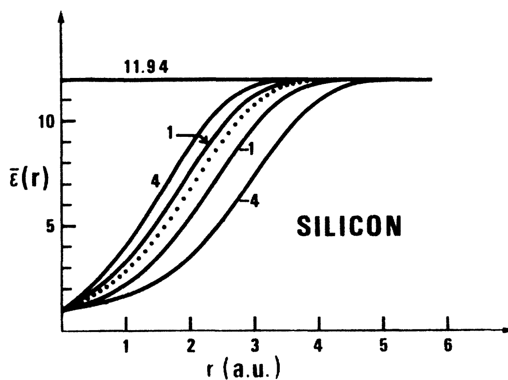

FIG. 2. Effective spatial dielectric constant for Si. The dotted line is the linear result, from Paper I.

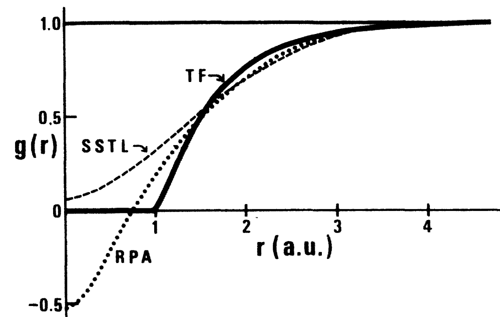

FIG. 4. $n(r)/n_0$ for $Z=-1$ in Si, solid line. The pair-correlation function of an electron gas at the same density is also shown. RPA, dashed line. STSL, Ref. 17, dotted line.

part, given by the difference between the core pseudopotentials of the impurity and of the host.

We point out that the present TF theory of nonlinear screening in semiconductors is by no means limited to the Coulomb potential (1). On the contrary, it can be straightforwardly generalized to any local bare impurity pseudopotential. We shortly outline here the route to be followed.

Given a local pseudopotential $V_0(r)$, one can easily find the classical electrostatic charge distribution which generates V_0. Then this charge distribution can be inserted in the Poisson equation of TF theory (2) [and eventually (4)] on the right-hand side, like an external rigid charge density. The whole procedure of Sec. II can be applied to the modified equations.

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