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Thomas-Fermi dielectric screening in semiconductors

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Thomas-Fermi (TF) screening in metals has been widely studied in the literature many years ago. It is shown in this paper that the same TF equation can be handled with different boundary conditions to describe screening in semiconductors. Explicit results for the wave-number-dependent dielectric function $\epsilon(\vec{k})$ and for the spatial dielectric function $\tilde{\epsilon}(\vec{r})$ are obtained in simple analytical form. A detailed comparison is done with the existing literature for diamond, Si, and Ge. TF dielectric functions are found to be in excellent agreement with either Penn model and random-phase approximation dielectric functions.

I. INTRODUCTION

A great deal of work has been devoted in the past to the wave-vector-dependent dielectric function $\epsilon(\vec{k})$ and to the spatial dielectric function $\tilde{\epsilon}(\vec{r})$ in semiconductors. The literature on the subject has become very extensive. The first model dielectric function has been proposed by Callaway[1]; this same model has been later refined by Tosatti and Pastori-Parravicini.[2] Another model dielectric function has been proposed by Penn[3] and evaluated more accurately by Srinivasan.[4] The Penn model has become very popular, and forms the basis of the Phillips–Van Vechten theory of ionicity in solids.[5] Refinements and modifications of the Penn model have been proposed,[6,7] as well as random-phase-approximation (RPA)[8] dielectric functions based on realistic band-structure calculations.[9-11] In this latter case, results have been found in excellent agreement with the simple Penn isotropic model.

$\epsilon(\vec{k})$ and $\tilde{\epsilon}(\vec{r})$ have many applications. They can be used to calculate vibrational spectra,[12] screened pseudopotential form factors,[13] electron-hole interaction in exciton problems[14] and impurity potentials.[15] It must be noted that even in the Penn model (and despite its conceptual simplicity) calculation of dielectric functions involves no little labor.[4] Simple analytical interpolation formulas [at least for $\epsilon(\vec{k})$] have been proposed in the literature,[3,4,16] in order to make applications easier.

We develop in this paper the Thomas-Fermi (TF) theory[17] of dielectric screening in semiconductors. The TF equation for impurity screening in metals was formulated long ago by Mott[18] and widely studied in the literature.[19-22] The new result of the present paper is that the same equation can be used to describe dielectric screening in semiconductors, by a suitable choice of boundary conditions.

The TF model dielectric functions $\epsilon(\vec{k})$ and $\tilde{\epsilon}(\vec{r})$ we propose in this paper are numerically found to be extremely close to Srinivasan's[4] Penn-model calculations. This is not surprising, since the TF degenerate-electron-gas approximation and the Penn model (nearly-free-electron gas with an energy gap) are conceptually very similar. The starting ingredients are also the same in our theory as in Penn's model, namely the static dielectric constant $\epsilon(0)$ and the Fermi momentum k_F.

There is however an important difference between the Penn model and the theory of the present paper. While calculation of Penn-model dielectric functions involves cumbersome integrations in $\vec{k}$ space,[4] TF-model dielectric functions $\epsilon(\vec{k})$ and $\tilde{\epsilon}(\vec{r})$ have a very simple analytical form, even simpler than the interpolation formulas proposed so far in the literature.[3,4,16]

In Sec. II we derive the TF equation for dielectric screening, following Mott.[18,22] In Sec. III the boundary conditions for semiconductor screening are discussed, in a framework suitable for any local-density scheme. In Sec. IV the TF equation is solved and the analytic expressions for the TF spatial dielectric function $\tilde{\epsilon}(\vec{r})$ and wave-vector-dependent dielectric function $\epsilon(\vec{k})$ are derived. In Sec. V results for diamond, Si, and Ge are explicitly shown and discussed by comparison with the existing literature.

II. TF EQUATION FOR POINT-CHARGE SCREENED POTENTIAL

We use throughout this paper atomic units $\hbar = 1$, $e^2 = 1$, $m_e = 1$. The whole theory we are going to develop is isotropic, and we drop the vector notations, since all quantities are functions of $|\vec{r}| = r$ and of $|\vec{k}| = k$. The model semiconductor is treated in the electron gas approximation, in the framework of TF theory. In the unperturbed solid of density n_0 = constant the electron momentum is uniformly distributed in $\vec{k}$-space within the Fermi sphere $k < k_F$, where

$$k_F = (3\pi^2 n_0)^{1/3} . \tag{1}$$

When a point-charge impurity potential

$$V_0(r) = \pm Z/r \tag{2}$$

is introduced in the electron gas, the charge density rearranges to screen V_0. Electrons are allowed to have higher kinetic energy where potential energy is lower and vice-versa. Classical condition of motion gives a relation between maximum momentum $k_{\max}(r)$ and self-consistent screened impurity potential $V(r)$, which we write as

$$\tfrac{1}{2}k^2_{\max}(r) + V(r) = \tfrac{1}{2}k_F^2 + A , \tag{3}$$

where A is a constant. The behavior of $k_{\max}(r)$ is schematically shown in Fig. 1. From the figure we also note that for repulsive $V(r)$ additional complications arise near $r = 0$, since $k_{\max}(r)$ cannot be negative. This difficulty can be overcome,[21,22] but for the sake of simplicity we consider in the following an attractive point-charge impurity, whose unscreened potential is

$$V_0(r) = -Z/r, \quad Z > 0 . \tag{4}$$

The TF equation for self-consistent screened potential $V(r)$ is easily established.[18,22] At point r, maximum allowed momentum is related to local density, as in (1).

$$k_{\max}(r) = (3\pi^2 n(r))^{1/3} . \tag{5}$$

From (5) and (3), and putting $E_F = \frac{1}{2}k_F^2$,

$$n(r) = (2^{3/2}/3\pi^2)[E_F + A - V(r)]^{3/2} . \tag{6}$$

Now the displaced electron density can be related to the screened potential by Poisson equation

$$-\nabla^2 V(r) = 4\pi[n(r) - n_0] , \tag{7}$$

and the final TF equation is

$$-\nabla^2 V(r) = (2^{7/2}/3\pi)\{[E_F + A - V(r)]^{3/2} - E_F^{3/2}\} . \tag{8}$$

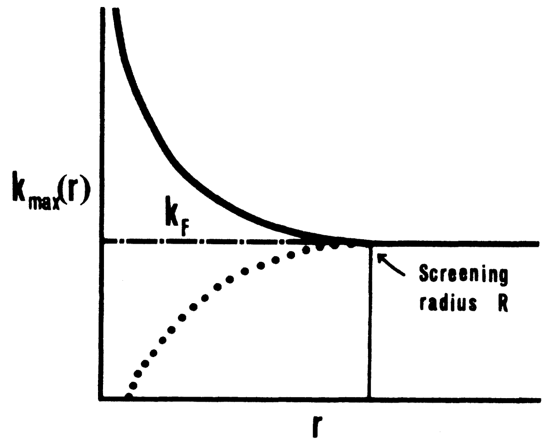

FIG. 1. Electron momentum distribution (schematic plot in arbitrary units). Dashed-dotted line: unperturbed solid; Solid line: point-charge attractive impurity; Dotted line: point-charge repulsive impurity.

As far as we are concerned with linear screening effects, Eq. (8) is linearized to

$$\nabla^2 V(r) = q^2[V(r) - A], \quad q = (4k_F/\pi)^{1/2} . \tag{9}$$

Equations (8) and (9) have been first established 40 years ago by Mott[18] and widely investigated later in the literature either in the linear and nonlinear form,[19,22] with the use of boundary conditions related to complete dielectric screening in metals.

The new result of the present paper is that, with the use of appropriate boundary conditions, these same equations are able to describe incomplete dielectric screening in semiconductors.

III. NATURE OF BOUNDARY CONDITIONS IN LOCAL-DENSITY THEORIES

In TF theory boundary conditions must be associated with Eq. (8) or (9). The first one is trivial: for either metals or semiconductors, $V(r)$ becomes unscreened for $r \to 0$, and the condition is

$$\lim_{r\to 0} rV(r) = \lim_{r\to 0} rV_0(r) = -Z . \tag{10}$$

The boundary condition at $r = \infty$ has, as we will show, deeper significance, and is related to the value of A in (8) or (9). The asymptotic behavior of $V(r)$ for $r \to \infty$ is related, by means of the Gauss theorem, to the total screening charge. The same happens in ordinary TF theory of atoms and ions, where the constraint is equivalent to assignment of ionic charge.

The constraint on the total number of particles which always arises in TF theories can be regarded from a more general point of view. If we consider, in fact, a system of interacting electrons in an external potential, total energy can be written within the TF approximation as a functional of local density. The Euler equation obtained by variation of this functional is in fact equivalent to the TF equation, and a constant like A in Eq. (8) and (9) is essentially the Lagrange multiplier related to the constraint on the total number of particles.

Equations (8) and (9) have been used so far to describe impurity screening in metals. The boundary condition at $r = \infty$ is in this case equivalent to assign the total number of displaced electrons equal to Z. The solution of this problem is $A = 0$ and, for the linear case (9)[18]

$$V(r) = -(Z/r)e^{-qr} = V_0(r)e^{-qr} . \tag{11}$$

We note here that TF screening in a metal extends over the whole crystal. In other words, the screening radius R of Fig. 1 is infinite.

Boundary condition at $r=\infty$ as given for a semiconductor yields a different result. It will be shown in Sec. IV that the incomplete screening charge in a semiconductor has finite radius R. We thus establish in this paper a complete analogy with the usual TF theory of atoms and ions.[17] It is well known, in fact, that in a TF atom the charge density extends over the whole space, while solutions of the same TF equation with boundary conditions as given for positive ions yield finite ionic radii.

We conclude this section noting that the above discussion on boundary conditions has a much more general validity than the TF approximation. The classical Hohenberg-Kohn theorem[23] states in fact that even in the exact many-body case the ground state energy can in principle be found by constrainted minimization of a (unique) functional of local density. The exact form of this functional is of course unknown, and TF scheme gives the simplest approximation to it. In the literature, accurate many-body results for the electron gas have been parametrized[24] to obtain local density functionals suitable for calculations.[25] A local density formalism has been very recently applied to the problem of point-charge screening in electron gas by Almbladth *et al.*[26] The boundary conditions used by these authors are, once more, related to complete screening in metals.

IV. SOLUTION OF THE TF EQUATION FOR LINEAR DIELECTRIC SCREENING

In the following of this paper we will refer only to linear screening and to the linearized Eq. (9). The boundary of the screening charge is defined through (see Fig. 1)

$$n(R)=n_0 \tag{12}$$

which gives for A, from (6), the relation

$$V(R)=A\,. \tag{13}$$

Beyond the screening radius R, the screened potential $V(r)$ of a point charge is given by

$$V(r)=-Z/\epsilon(0)r,\quad r\geq R, \tag{14}$$

where $\epsilon(0)$ is the static dielectric constant. Inside the screening radius the potential is described by Eq. (9), whose general solution we write as

$$V(r)=-(Z/r)(\alpha e^{qr}+\beta e^{-qr})+A,\quad r<R\,. \tag{15}$$

By imposing continuity at $r=R$, and using (10) and (13), Eq. (15) is finally rewritten

$$V(r)=-\frac{Z}{r}\,\frac{\sinh q(R-r)}{\sinh qR}-\frac{Z}{\epsilon(0)R},\quad r\leq R\,. \tag{16}$$

The screening radius R is found by imposing continuity of electric field at $r=R$. Taking the derivatives of (14) and (16) and equating we obtain

$$\sinh qR/qR=\epsilon(0)\,. \tag{17}$$

This equation yields a finite solution for R for any $\epsilon(0)>1$. The metallic case formally corresponds to $\epsilon(0)=\infty$, and we obtain in this case $R=\infty$, in agreement with expression (11).

If we introduce the spatial dielectric function $\bar{\epsilon}(r)$, defined by

$$V(r)=-Z/r\bar{\epsilon}(r)\,, \tag{18}$$

the results (14) and (16) are rewritten as

$$\bar{\epsilon}(r)=\begin{cases}\epsilon(0)qR/[\sinh q(R-r)+qr]\,, & r\leq R\\ \epsilon(0), & r\geq R\,.\end{cases} \tag{19}$$

The spatial dielectric function $\bar{\epsilon}(r)$, which is defined in (18) following the current usage in literature[4,10,16] is useful only in the very special case of a point-charge external disturbance. The linear response to an arbitrary external probe is in fact nonlocal, and must be expressed in terms of a convolution integral.

On the other hand, the linear response of a homogeneous system is local in $\vec{k}$ space. The wave-vector-dependent dielectric function is defined through the Fourier transforms of the screened and unscreened potentials

$$1/\epsilon(k)=\tilde{V}(k)/\tilde{V}_0(k)\,, \tag{20}$$

and the same $\epsilon(k)$ applies to any external potential $\tilde{V}_0(k)$. We actually know the linear response to a point-charge probe, so that $\epsilon(k)$ can be determined from (20), taking the transforms of (4) and (14), (16). This can be performed exactly, and the final result is

TABLE I. Summary of relevant figures for diamond, Si, and Ge.

	Diamond	Silicon	Germanium
Nearest-neighbor distance (a.u.)	2.91	4.44	4.63
Valence Fermi momentum k_F (a.u.)	1.46	0.96	0.92
$q=(4k_F/\pi)^{1/2}$	1.36	1.10	1.08
Static dielectric constant ϵ (0)	5.7	11.94	16.0
Screening radius R (a.u.), from Eq. (17)	2.76	4.28	4.71

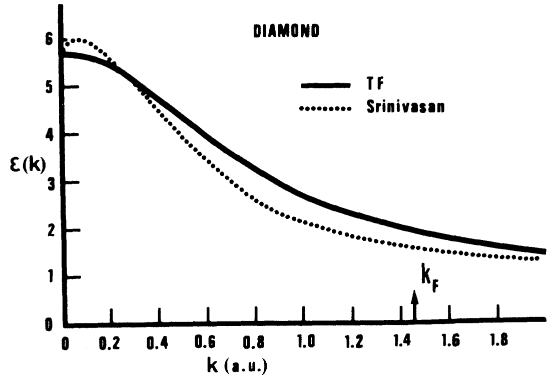

FIG. 2. Wave-vector-dependent dielectric function in diamond. Solid line: this work (TF); Dotted line: Ref. 4 (isotropic Penn model).

$$\epsilon(k) = \frac{q^2 + k^2}{[q^2/\epsilon(0)]\sin kR/kR + k^2}\,. \tag{21}$$

The TF dielectric functions we propose in the present paper are easily obtainable for any semiconductor. The only input data needed are the static dielectric constant $\epsilon(0)$ and the valence Fermi momentum k_F, as in Penn model.[3,4] R is found by solution of (17) and the final results have the quite simple analytical expressions (19) and (21). It should be noted that the TF theory of the present paper gives an $\vec{r}$-space model dielectric screening, while Penn model is essentially a $\vec{k}$-space model theory. Although conceptually the two models are very close, the amount of computation needed is quite different. The final results, on the other side, are quite similar. A detailed comparison is done for diamond, Si, and Ge in Sec. V.

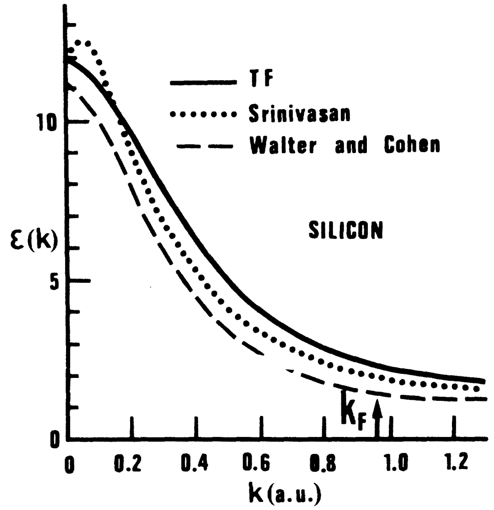

FIG. 3. Wave-vector-dependent dielectric function in Si. Solid line: this work (TF); Dotted line: Ref. 4 (isotropic Penn model); Dashed line: Ref. 11 [RPA along (1,0,0)].

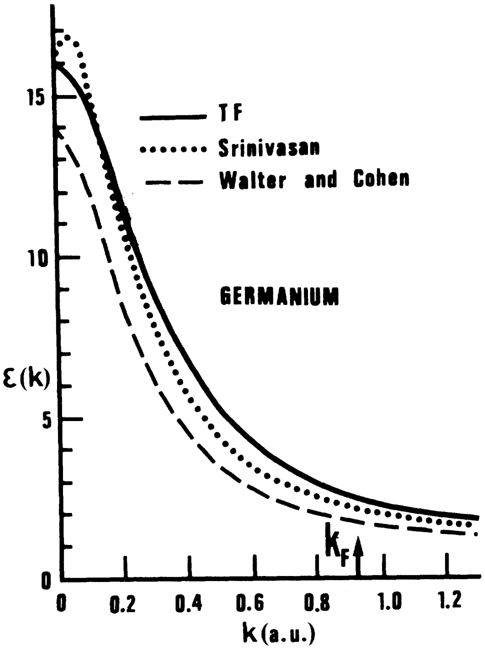

FIG. 4. Wave-vector-dependent dielectric function in Ge. Solid line: this work (TF); Dotted line: Ref. 4 (isotropic Penn model); Dashed line: Ref. 11 [RPA along (1,0,0)].

V. RESULTS FOR DIAMOND, SILICON, AND GERMANIUM

A number of different calculations of the wave-vector-dependent dielectric function $\epsilon(k)$ exists in the literature for Si and Ge.[2-4,9-11] These calculations in most cases closely match Srinivasan's[4] Penn-model results.

The TF wave-vector-dependent dielectric functions $\epsilon(k)$ for diamond, Si, and Ge have been eval-

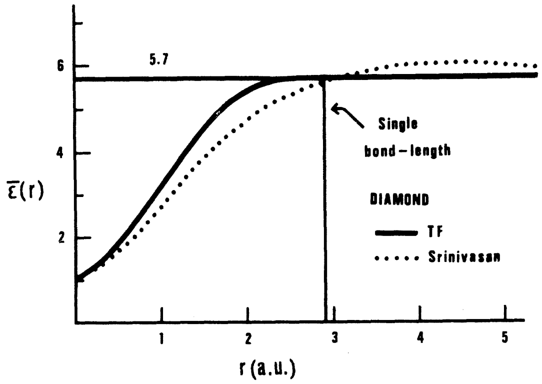

FIG. 5. Spatial dielectric function in diamond. Solid line: this work; Dotted line: Ref. 4.

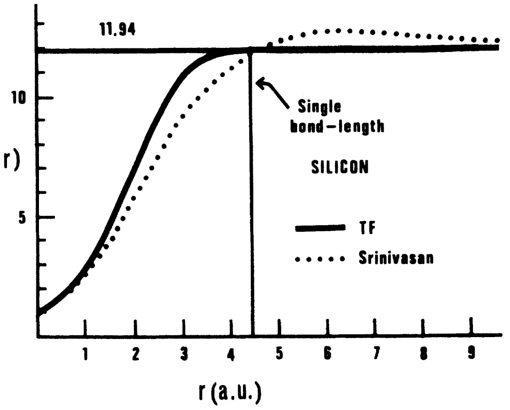

FIG. 6. Spatial dielectric function in Si. Solid line: this work; Dotted line: Ref. 4.

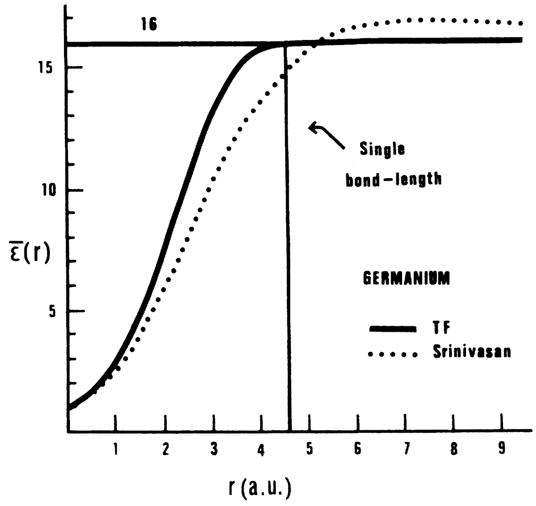

FIG. 7. Spatial dielectric function in Ge. Solid line: this work; Dotted line: Ref. 4.

uated from expression (21). The values of the static dielectric constants $\epsilon(0)$ and of the valence Fermi momentum k_F used are shown in Table I. The values of screening radii R, defined by equation (17), are also reported in the table. The resulting $\epsilon(k)$ are shown in Figs. 2–4, together with isotropic Penn-model results of Srinivasan[4] and RPA results of Walter and Cohen[11] along the direction (1, 0, 0). It is easily seen that the agreement is excellent, despite the extreme simplicity of the analytic expression (21).

A remark should be made about the low-wave-number behavior of $\epsilon(k)$. The TF dielectric function of the present paper is monotonically decreasing, while Srinivasan's calculation shows a maximum at $k \simeq 0.05k_F$. In the framework of Penn's model, the low-k behavior results from a delicate cancellation of "normal" and "umklapp" terms,[4] so that no physical meaning should be attached to these maxima. As a matter of fact, the accurate pseudopotential RPA calculation of Walter and Cohen[11] in Si and Ge yields nearly isotropic $\epsilon(\vec{k})$, which is (over a given direction) monotonical and numerically quite close to the present TF results.

The TF spatial dielectric functions $\bar{\epsilon}(r)$ for diamond, Si, and Ge evaluated from expression (19) are reported in Figs. 5–7. As shown in the preceding section, the spatial screening charge has finite range R. Numerical values for R obtained from Eq. (17) are very close to the nearest-neighbor distance in the crystal, as reported in Table I and in the figures.

As already noted, dielectric screening in semiconductors is evaluated by the authors quoted above[1–4,6–11] in $\vec{k}$ space, and then is sometimes transformed to $\vec{r}$ space,[4,10,16] while in the TF theory of the present paper one first finds $\bar{\epsilon}(r)$ and then $\epsilon(k)$. A study of $\bar{\epsilon}(r)$ in diamond, Si, and Ge has been performed by Srinivasan,[4] with the aid of an interpolation formula for $\epsilon(k)$. These results are also shown in Figs. 5–7; they are, as expected, close to ours.

In particular, Srinivasan obtains that $\bar{\epsilon}(r)$ is approximately equal to $\epsilon(0)$ beyond a distance close to the single-bond length, while in the theory of the present paper $\bar{\epsilon}(r) = \epsilon(0)$ exactly for $r \geq R$. The overshoot in $\bar{\epsilon}(r)$ over $\epsilon(0)$ for large r is probably a numerical artifact, as already noted by the same author[4] and by Vinsome and Richardson.[10] The TF theory is probably better than the Penn model in this respect.

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