Asymptotic forms of electrostatic potentials in zero-band-gap semiconductors: Bulk versus surface screening

L. R. González
Departamento de Física, Facultad de Ciencias, Universidad de Los Andes, Mérida 5101, Venezuela

J. Krupski
Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, PL-00-681 Warsaw, Poland

T. Szwacka
Departamento de Física, Facultad de Ciencias, Universidad de Los Andes, Mérida 5101, Venezuela
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In this paper we calculate the asymptotic forms of the screened electrostatic potentials in both bulk and semi-infinite zero-band-gap semiconductors, which are described with the help of a random-phase approximation dielectric function. We consider the effective potential of a point charge as well as the screening of a uniform electric field. We show how, in comparison with the free-electron-gas case, the amplitudes of Friedel oscillations of the effective potentials are considerably reduced due to the specific band structure of the gapless materials. To analyze the surface screening, we use the specular electron reflection model. The long- and short-range forms of the potentials obtained in the framework of various asymptotic methods agree with the results of computer calculations.

I. INTRODUCTION

The shape of the screened electrostatic potential in both bulk and semi-infinite solids plays an important role in various physical problems such as impurity levels, adatom interaction, and field emission to mention only a few. In the bulk material this potential is given by the Fourier integral

$$V(\mathbf{r})=\int \frac{d^3q}{(2\pi)^3}\frac{V_{\rm ext}(\mathbf{q})}{\epsilon(\mathbf{q})}\exp(i\mathbf{q}\cdot\mathbf{r})\ , \tag{1}$$

where $V_{\rm ext}$ is an external potential. $V_{\rm ext}(\mathbf{q})=4\pi Q_{\rm ext}q^{-2}$ for a point charge $Q_{\rm ext}$ inserted into the system. $\epsilon(\mathbf{q})$ is the longitudinal dielectric function. This function can be obtained in the random-phase approximation (RPA) which in the case of degenerate free-electron gas leads to the well-known Lindhard formula[1]

$$\epsilon(\mathbf{q})=\epsilon_0+\frac{1}{2}\left[\frac{k_{\rm TF}}{k_F}\right]^2\left[\frac{k_F}{q}\right]^2 \times\left[1+\frac{k_F}{q}\left[1-\frac{q^2}{4k_f^2}\right]\ln\left|\frac{1+\frac{q}{2k_F}}{1-\frac{q}{2k_F}}\right|\right], \tag{2}$$

where ϵ_0 is the static dielectric constant, k_F and $k_{\rm TF}$ are the Fermi and the Thomas-Fermi wave numbers, respectively. If the concentration of the electrons is n, then $k_F=(3\pi^2n)^{1/3}$. $k_{\rm TF}=(4k_F/\pi a_0)^{1/2}$, where $a_0=\hbar^2/me^2$ is the Bohr radius.

Integral (1) with $\epsilon(\mathbf{q})$ given by (2) and with $v_{\rm ext}(\mathbf{q})=4\pi Q_{\rm ext}q^{-2}$ is too difficult to be performed analytically; however, its asyptotic form for large $|\mathbf{r}|$ can be derived from the algebraico-logarithmic singularity of $\epsilon(\mathbf{q})$ at $2k_F$. Finally, as it was shown by Langer and Vosko,[2] $V(\mathbf{r})$ oscillates as $\cos 2k_Fr/r^3$ (Friedel oscillations[3]).

The results for nonspherical Fermi surfaces were given by Roth, Zeiger, and Kaplan[4] and by Gabovich *et al.*[5] Horing studied the influence of the magnetic field on Friedel oscillations in an electron gas.[6]

Friedel oscillations of the screened uniform electrostatic field in a semi-infinite metal were studied comprehensively by Balkarei and Sandomirsky.[7] Dielectric response of a semi-infinite metal was also investigated by Newns[8] and Beck *et al.*[9,10] and Sidyakin[11] and Rudnick.[12]

Recently the measurement of the adatoms interaction on a metal surface by Tsong and Casanova[13,14] has highlighted again the importance of the screening in semi-infinite solids. Oscillatory behavior of the interaction energy between adatoms was investigated theoretically by Grimley and Walker,[15] Einstein and Schrieffer,[16] Lau and Kohn,[17] Kravtsov,[18] and by Braun and Il'chenko and Pashitskii.[19] Electron potential energy near the surface of a ferromagnetic metal was calculated by Gabovich and Voitenko.[20]

Whereas the majority of the papers mentioned above deal with the metals, we wish to focus our attention on semiconductors. It is the purpose of this paper to investigate the influence of the electronic band structure on asymptotic forms of the effective Coulomb potential and of the screened uniform electric field in both bulk and semi-infinite zero-gap semiconductors. The calculations of the potential in a semi-infinite semiconductor are based

on the so-called specular electron reflection model (see, for example, Ref. 21) which is described in detail in Ref. 22.

The long- and short-range forms of the potentials obtained with the help of various asymptotic methods are confirmed by computer calculations.

II. SCREENING IN THE BULK

Usually RPA longitudinal dielectric function $\epsilon(\mathbf{q})$ of a semiconductor is written as a sum of ϵ_0, $\epsilon^{\text{inter}}(\mathbf{q})$, and $\epsilon^{\text{intra}}(\mathbf{q})$, where the last two terms are due to the transitions between valence and conduction bands and within conduction bands, respectively. All other contributions to $\epsilon(\mathbf{q})$, including lattice polarizability, are approximated by the dielectric constant ϵ_0.

The dielectric function for gapless semiconductors with nonvanishing concentration of free carriers was known in the form of an infinite series since the 70s.[23–25] Recently it was shown[26] that one can express $\epsilon(\mathbf{q})$ for zero-gap materials in a compact form by using Euler's dilogarithms (see, for example, Ref. 27), i.e., $L_2(z)=-\int_0^z d\xi (1/\xi)\ln(1-\xi)$. Finally, in the limit $m_h/m_e \to \infty$, the result is as follows:[26]

$$\epsilon(\mathbf{q})=\epsilon_0+\frac{3}{4}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{k_F}{q}\right]^2\left\{\frac{2}{3}+\frac{1}{2}\left[\frac{q}{k_F}\right]^2+\frac{2}{3}\frac{k_F}{q}\left[1+\frac{3}{4}\left[\frac{q}{k_F}\right]^2\right]\left[1-\frac{1}{4}\left[\frac{q}{k_F}\right]^2\right]\ln\left|\frac{1+\frac{q}{2k_F}}{1-\frac{q}{2k_F}}\right|\right.$$
$$\left.+\frac{q}{k_F}\left[L_2\left[\frac{q}{2k_F}\right]-L_2\left[-\frac{q}{2k_F}\right]\right]\right\}. \tag{3}$$

The source of singularities in $\epsilon(\mathbf{q})$ given by (3) are the terms with the logarithmic function and with Euler's dilogarithms. We checked that the position of these singularities ($q=\pm 2k_F$) and theory type (algebraico-logarithmic) are the same as those of Lindhard dielectric function (2). Generally, the behavior of the dielectric functions (2) and (3) near the singularity at $q=2k_F$ is

$$\epsilon(q)\cong\epsilon(2k_F)\left[1+D\epsilon(2k_F)\left[\frac{q}{k_F}-2\right]\ln\left|\frac{q}{k_F}-2\right|\right], \tag{4}$$

where

$$\epsilon(2k_F)=\epsilon_0+\tfrac{1}{8}(k_{\text{TF}}/k_F)^2, \tag{5}$$

$$D=\frac{1}{16}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\epsilon_0+\frac{1}{8}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\right]^{-2} \tag{6}$$

for free electrons characterized with the Lindhard dielectric function. In the case of the gapless semiconductor one has

$$\epsilon(2k_F)=\epsilon_0+\tfrac{1}{2}(1+3\pi^2/16)(k_{\text{TF}}/k_F)^2, \tag{7}$$

$$D=\frac{1}{16}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\epsilon_0+\frac{1}{2}\left[1+\frac{3\pi^2}{16}\right]\left[\frac{k_{\text{TF}}}{k_F}\right]^2\right]. \tag{8}$$

We turn now to the screened potential $V_b(\mathbf{r})$ of a point charge Q_{ext} located in the bulk at $\mathbf{r}=0$. According to (1) V_b may be written as ($\xi=q/k_F$, where H is the step function)

$$V_b(\mathbf{r})=\frac{2}{\pi}Q_{\text{ext}}k_F\frac{1}{k_F r}\,\text{Im}\int d\xi\, H(\xi)\frac{\exp(i\xi k_F r)}{\xi\epsilon(\xi k_F)}. \tag{9}$$

This integral is too difficult to be performed analytically when ϵ is given by (2) or (3). To find its asymptotic form for $k_F r\gg 1$, we employ the technique presented by Lighthill.[28] The leading terms in the asymptotic expansion of (9) can be obtained from the singularity of the integrand at $\xi=2$, where $1/\epsilon$ can be simplified to

$$1/\epsilon(2k_F)-D(\xi-2)\ln|\xi-2|$$
$$+D^2\epsilon(2k_F)(\xi-2)^2\ln^2|\xi-2|+\cdots.$$

The final result for $k_F r\gg 1$ is

$$V_b(\mathbf{r})\cong Q_{\text{ext}}k_F\left[D\frac{\cos(2k_F r)}{(k_F r)^3}\right.$$
$$-4D^2\epsilon(2k_F)[\ln(k_F r)+\psi(2)]$$
$$\left.\times\frac{\sin(2k_F r)}{(k_F r)^4}+\cdots\right]. \tag{10}$$

where $\epsilon(2k_F)$ and D are given by (5) and (6) for free electrons and by (7) and (8) for zero-gap semiconductors.

III. SURFACE SCREENING

A. Model

We assume here that the semiconductor occupies the $z<0$ region and that the interface vacuum semiconductor is the $z=0$ plane. To find the screened potential $V(\mathbf{r})$ of an extra point charge in the system semiconductor vacuum, we make use of the specular electron reflection model (see, for example, Ref. 21 where this

model is named classical infinite barrier model although it is not classical). If the positions of the observer and the extra point charge Q_{ext} are $\mathbf{r}=(\zeta,z)$ and $\mathbf{r}_0=(\zeta=0,z_0)$, respectively, then (see, for example, Ref. 22)

$$V(\mathbf{r})=\frac{1}{2\pi}\int_0^\infty dq_\parallel q_\parallel J_0(q_\parallel\zeta)v_s(q_\parallel,z,z_0)\ , \tag{11}$$

where

$$\begin{aligned}v_s(q_\parallel,z,z_0)=\frac{2\pi Q_{\text{ext}}}{q_\parallel}\Bigg[&H(z)H(z_0)\left[\exp(-q_\parallel|z-z_0|)-\frac{1-a(q_\parallel,0)}{1+a(q_\parallel,0)}\exp[-q_\parallel(z+z_0)]\right]\\&+H(z)H(-z_0)\frac{2a(q_\parallel,z_0)\exp(-q_\parallel z)}{1+a(q_\parallel,0)}+H(-z)H(z_0)\frac{2a(q_\parallel,z)\exp(-q_\parallel z_0)}{1+a(q_\parallel,0)}\\&+H(-z)H(-z_0)\left[a(q_\parallel,z-z_0)+a(q_\parallel,z+z_0)-\frac{2a(q_\parallel,z)a(q_\parallel,z_0)}{1+a(q_\parallel,0)}\right]\Bigg]\end{aligned} \tag{12}$$

and

$$\zeta=(x^2+y^2)^{1/2}$$

since

$$\zeta=(x,y),\quad q_\parallel=(q_x^2+q_y^2)^{1/2},\quad q_\perp=q_z\ , \tag{13}$$

$$a(q_\parallel,z)=\frac{2}{\pi}q_\parallel\int_0^\infty dq_\perp\frac{\cos(q_\perp z)}{q^2\epsilon(q)}\ .$$

Here $\epsilon(q)$ is the dielectric function that characterizes the bulk semiconductor. In determining the properties of the function $a(q_\parallel,z)$ it is convenient to write (13) as

$$a(q_\parallel,z)=\frac{2}{\pi}q_\parallel\int_{q_\parallel}^\infty dq\frac{\cos[(q^2-q_\parallel^2)^{1/2}z]}{(q^2-q_\parallel^2)^{1/2}q\epsilon(q)}\ . \tag{14}$$

In particular, $a(q_\parallel,0)$ for large $q_\parallel$ can be obtained by inserting in (14) the asymptotic form of $\epsilon(q)$ when q tends to infinity. Noting the Lindhard dielectric function

$$\epsilon(q)\to\epsilon_0+\frac{4}{3}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q}{k_F}\right]^{-4}+\frac{16}{15}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q}{k_F}\right]^{-6}+\cdots \tag{15}$$

as $q\to\infty$, one gets that for free electrons

$$a(q_\parallel,0)\to\frac{1}{\epsilon_0}-\frac{1}{2\epsilon_0^2}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q_\parallel}{k_F}\right]^{-4}-\frac{1}{3\epsilon_0^2}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q_\parallel}{k_F}\right]^{-6}+\cdots \tag{16}$$

as $q_\parallel\to\infty$. The corresponding results for gapless semiconductors are

$$\epsilon(q)\to\epsilon_0+\frac{3\pi^2}{8}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q}{k_F}\right]^{-1}-2\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q}{k_F}\right]^{-2}+\cdots \tag{17}$$

and

$$a(q_\parallel,0)\to\frac{1}{\epsilon_0}-\frac{3\pi}{4\epsilon_0^2}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q}{k_F}\right]^{-1}+\frac{1}{\epsilon_0^2}\left[1+\frac{9\pi^4}{128\epsilon_0}\left[\frac{k_{\text{TF}}}{k_F}\right]^2\right]\times\left[\frac{k_{\text{TF}}}{k_F}\right]^2\left[\frac{q}{k_F}\right]^{-2}+\cdots \tag{18}$$

as $q,q_\parallel\to\infty$.

Small q limit form of $\epsilon(\mathbf{q})$ (Thomas-Fermi approximation) is $\epsilon^{\text{TF}}(q)=\bar{\epsilon}_0+(k_{\text{TF}}/q)^2$, where $\bar{\epsilon}_0=\epsilon_0-(k_{\text{TF}}/k_F)^2/12$ for free electrons and $\bar{\epsilon}_0=\epsilon_0+17(k_{\text{TF}}/k_F)^2/12$ for gapless semiconductors. In this case the analytical form of a is known as

$$a^{\text{TF}}(q_\parallel,z)=\frac{q_\parallel\exp[-z(q_\parallel^2+k_{\text{TF}}^2/\bar{\epsilon}_0)^{1/2}]}{\bar{\epsilon}_0(q_\parallel^2+k_{\text{TF}}^2/\bar{\epsilon}_0)^{1/2}}\ . \tag{19}$$

Let us note that V_b given by (9), i.e., the screened point-charge potential in the bulk can be expressed by (11) with $v_s(q_\parallel,z,z_0)=2\pi Q_{\text{ext}}a(q_\parallel,z)/q_\parallel$. This suggests [see also Eqs. (11) and (12)] that deep inside semi-infinite solid ($z,z_0<0$)

$$V(\mathbf{r})\cong V_b(\zeta,z-z_0)+V_b(\zeta,z+z_0)\ , \tag{20}$$

when

$$k_F|z|,\ k_F|z_0|\gg 1\ .$$

B. The case where both the observer and Q_{ext} are in the vacuum

In this case $z,z_0\geq 0$. We wish to calculate the induced potential $V_{\text{ind}}(\mathbf{r},z_0)$, so we skip in (12) the term proportional to $\exp(-q_\parallel|z-z_0|)$ which corresponds to the pure Coulomb potential. The remaining term is proportional to $\exp[-q_\parallel(z-z_0)]$ and integral (11) may be interpreted as a Laplace transform

$$V_{\text{ind}}(\mathbf{r},z_0)=-Q_{\text{ext}}\int_0^\infty dq_\parallel J_0(q_\parallel\zeta)\frac{1-a(q_\parallel,0)}{1+a(q_\parallel,0)}\times\exp[-q_\parallel(z+z_0)]\ . \tag{21}$$

Asymptotic expansion of $V_{\text{ind}}(\mathbf{r},z_0)$ for large $z+z_0$ is given by (21) with the integrand simplified to its small-q limit form. Hence it follows that for $k_F(z+z_0)\gg 1$

$$V_{\text{ind}}(\mathbf{r},z_0)\cong -Q_{\text{ext}}k_F\frac{1}{[(k_F\zeta)^2+k_F^2(z+z_0)^2]^{1/2}} +2Q_{\text{ext}}k_F\frac{k_F(z+z_0)}{[(k_F\zeta)^2+k_F^2(z+z_0)^2]^{3/2}} \times\left[\frac{a(q_\parallel,0)}{q_\parallel/k_F}\right]_{q_\parallel=0}+\cdots . \tag{22}$$

The leading term in the expansion is nothing more than the image-force potential of the classical metal. The remaining part is the quantum correction.

$V_{\text{ind}}(\mathbf{r},z_0)$ is divergent when $\mathbf{r},z_0=0$ which follows from the long-range behavior of the integrand in (21). From (16) and (18) it can be deduced that when $q_\parallel$ is large, then

$$\frac{1-a(q_\parallel,0)}{1+a(q_\parallel,0)}\cong\frac{\epsilon_0-1}{\epsilon_0+1}+O\left[\frac{1}{q_\parallel^4}\right] \tag{23}$$

for free electrons and

$$\frac{1-a(q_\parallel,0)}{1+a(q_\parallel,0)}\cong\frac{\epsilon_0-1}{\epsilon_0+1}+\frac{3\pi}{2}\left[\frac{k_{\text{TF}}/k_F}{\epsilon_0+1}\right]^2\frac{k_F}{q_\parallel}+O\left[\frac{1}{q_\parallel^2}\right] \tag{24}$$

for gapless semiconductors. To extract the singular term in V_{ind} when $\mathbf{r},z_0=0$ let us write for free electrons

$$\frac{1-a(q_\parallel,0)}{1+a(q_\parallel,0)}=\frac{1-a(q_\parallel,0)}{1+a(q_\parallel,0)}-\frac{\epsilon_0-1}{\epsilon_0+1}+\frac{\epsilon_0-1}{\epsilon_0+1} . \tag{25}$$

Now one can see that the only source of the divergency in (21) when $\mathbf{r},z_0$ tend to zero is the last term in (25). Finally, in the free-electron-gas case when $\mathbf{r},z_0$ tend to zero we get

$$V_{\text{ind}}(\mathbf{r},z_0)\cong -Q_{\text{ext}}k_F\frac{(\epsilon_0-1)/(\epsilon_0+1)}{[(k_F\zeta)^2+k_F^2(z+z_0)^2]^{1/2}}+\cdots . \tag{26}$$

In contrast to (25) in the zero-gap semiconductor case we subtract and add to $(1-a)/(1+a)$ two terms:

$$(\epsilon_0-1)/(\epsilon_0+1)+(3\pi/2)[(k_{\text{TF}}/k_F)/(\epsilon_0+1)]^2 \times(k_F/q_\parallel)\exp(-bk_F/q_\parallel) ,$$

which are the source of the divergent parts in V_{ind} (b is an arbitrary strictly positive constant introduced in order to make the appropriate integral finite). Finally, keeping only singular terms for $\mathbf{r},z_0\to 0$, we get the following result for the gapless semiconductors:

$$V_{\text{ind}}(\mathbf{r},z_0)\cong -Q_{\text{ext}}k_F\frac{(\epsilon_0-1)/(\epsilon_0+1)}{[(k_F\zeta)^2+k_F^2(z+z_0)^2]^{1/2}} +Q_{\text{ext}}k_F\frac{3\pi}{2}\left[\frac{k_{\text{TF}}/k_F}{\epsilon_0+1}\right]^2\ln\{[(k_F\zeta)^2+k_F^2(z+z_0)^2]^{1/2}+k_F(z+z_0)\}+\cdots . \tag{27}$$

In both situations [Eqs. (26) and (27)] the leading terms are equal to the results for the classical dielectric. In the zero-gap semiconductor case there is an additional, singular term of logarithmic type.

Figures 1 and 2 show $V_{\text{ind}}(\zeta=0,z,z_0=z)$ i.e., V_{ind} at the external point-charge site for CdS ($\epsilon_0=9.38$) and for the gapless semiconductor HgTe ($\epsilon_0=21$), respectively. Conduction-band electrons in open-gap material CdS are represented by free-electron gas with appropriate effective mass of the carriers. $V_{\text{ind}}(\zeta=0,z,z_0=z)/2$ can be interpreted as the potential felt, say, by an electron ($Q_{\text{ext}}=e$) that left the solid. As it follows from our considerations this potential is equal to a classical dielectric close to the semiconductor surface and tends to equal the classical metal at large distances.

C. The case where the observer and Q_{ext} are separated by the semiconductor surface

Now $zz_0<0$. $V(\mathbf{r})$ is given by the double integral. One of these integrals is a Laplace transform which we treat as that in the preceding section. The remaining integral is of the form discussed by Lighthill.[28] When $k_F|z|,k_F|z_0|\gg 1$, the final result for $V(\mathbf{r})$ appears as [$\mathbf{r}=(\zeta,z)$]

$$V(\mathbf{r},z_0)\cong V_1(\zeta,z,z_0)+V_1(\zeta,z_0,z) , \tag{28}$$

where

$$V_1(\zeta,z,z_0)=-Q_{\text{ext}}k_FD\frac{k_Fz}{[(k_F\zeta)^2+(k_Fz)^2]^{3/2}} \times\frac{\sin(2k_F|z_0|)}{(k_Fz_0)^2}H(z)H(-z_0) .$$

D is given by (6) or (8). Note that to get this result we evaluated the Laplace transform first.

D. The case where both the observer and Q_{ext} are on the surface

Now $z=z_0=0$. According to (11) the potential V is

$$V(\zeta)=2Q_{\text{ext}}\int_0^\infty dq_\parallel\frac{a(q_\parallel,0)}{1+a(q_\parallel,0)}J_0(q_\parallel\zeta) . \tag{29}$$

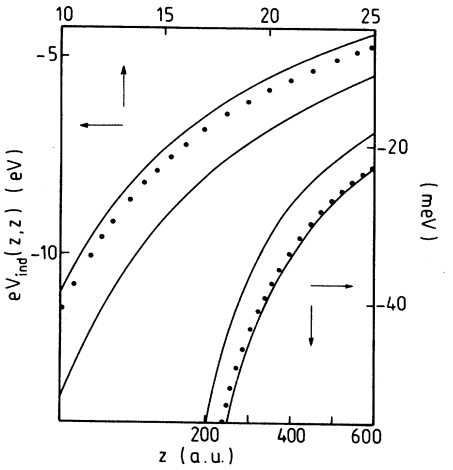

FIG. 1. Long- and short-range behavior of $eV_{\rm ind}(z,z_0=z)$ (i.e., the induced potential at the site of the external point charge which is located outside the semiconductor) for CdS when $n=10^{17}$ cm^{-3} ($\epsilon_0=9.38, m_e=0.2m_0$). In both groups of the curves upper and lower solid lines show the results for the classical dielectric and metal, respectively. Computer calculations according to Eq. (21) are represented by the dots. Arrows indicate to which scale the groups of the curves are related.

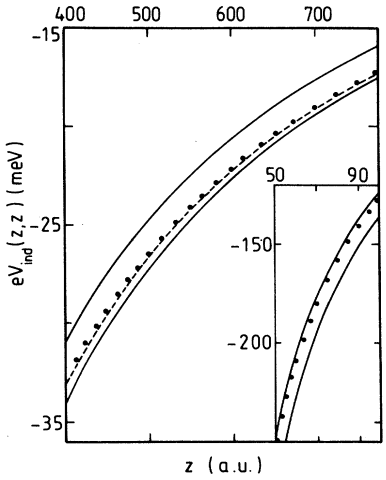

FIG. 2. Long- and short-range behavior of $eV_{\rm ind}(z,z_0=z)$ (i.e., the induced potential at the site of the external point charge which is located outside the semiconductor) for HgTe when $n=10^{17}$ cm^{-3} ($\epsilon_0=21, m_e=0.03m_0$). On both parts of the picture upper and lower solid lines show the results for the classical dielectric and metal, respectively. Computer calculations according to Eq. (21) are represented by the dots. The dashed line comes from the asymptotic form (22).

$V(\zeta)$ for small $k_F\zeta$ can be obtained by adding to (26) or (27) the pure Coulomb term $Q_{\rm ext}/\zeta$.

To find an asymptotic form of $V(\zeta)$ for $k_F\zeta \gg 1$, we follow the method used by Kravtsov[18] (contour integration) introducing necessary modifications due to specific forms of the dielectric function for gapless semiconductors. As it follows from Ref. 18 the asymptotic form of $V(\zeta)$ for free electrons consists of two parts V_n and V_0 of nonoscillatory and oscillatory characters, respectively, which decay as ζ^{-3} [the result for $V(\zeta)$ given in Ref. 5 is wrong]. The nonoscillatory term is

$$V_n(\zeta)=2Q_{\rm ext}k_F\left[\frac{a(q_\parallel,0)}{q_\parallel/k_F}\right]^2_{q_\parallel=0}\frac{1}{(k_F\zeta)^3} \tag{30}$$

and can be derived in the same way for free electrons as well as for zero-gap semiconductors.

To find oscillatory contribution to the asymptotic form of $V(\zeta)$, let us write in the expressions for the dielectric functions that $\ln|\xi/2\pm1|=\lim_{\eta\to0}\frac{1}{2}\ln[(\xi/2\pm1)^2+\eta^2/4]$. We choose $2+ip+i\eta, 0\le p<\infty$ as a cut in a complex ξ plane for $\ln(\xi/2-1-i\eta/2)$ as well as for $L_2(\xi/2)$ which appears in the gapless semiconductor case. As it was shown in Ref. 18 the oscillatory part $V_0(\zeta)$ of the potential $V(\zeta)$ can be written as

$$V_0(\zeta)=2Q_{\rm ext}k_F\,{\rm Re}\,i\int_0^\infty dt\,H_0^{(1)}(2k_F\zeta+ik_F\zeta t)A(t)\ , \tag{31}$$

where $A(t)=A^+(t)-A^-(t)$ and $A^\pm(t)=a^\pm(k_F(2+it),0)[1+a^\pm(k_F(2+it),0)]^{-1}$. Here $a^\pm(k_F(2+it),0)=\lim_{\delta\to+0}a(k_F(2^\pm\delta+it),0)$, where a is given by (13). Using the behavior of Hankel function of the first kind $H_0^{(1)}$ when $k_F\zeta\gg1$, we can replace $A(t)$ in (31) by its small t limit form which is

$$A(t)\cong\frac{a^+(k_F(2+it),0)-a^-(k_F(2+it),0)}{[1+a(2k_F,0)]^2}\ . \tag{32}$$

As it follows from Ref. 18 the numerator in (32) can be written as [see also Eq. (14)]

$$a^+(k_F(2+it),0)-a^-(k_F(2+it),0)=\int_C d\xi\frac{1/\xi}{(\xi^2-\xi_\parallel^2)^{1/2}}\left[\frac{1}{\epsilon^+(\xi k_F)}-\frac{1}{\epsilon^-(\xi k_F)}\right], \tag{33}$$

where the contour C is $2+it'$, $0\le t'\le t$. For small t

$$\frac{1}{\epsilon^+(\xi k_F)}-\frac{1}{\epsilon^-(\xi k_F)}\cong\frac{\epsilon^-(\xi k_F)-\epsilon^+(\xi k_F)}{\epsilon^2(2k_F)}\ . \tag{34}$$

$\epsilon^--\epsilon^+$ is the difference between the values of ϵ taken on both sides of the contour C in (33). This difference comes form the logarithmic term in the free-electron-gas case and from logarithm and Euler's dilogarithm in the case of gapless semiconductors. The difference on both sides of the cut C in the case of the logarithm is

$$\tfrac{1}{2}\lim_{\eta\to+0}\{\ln^-[\xi-(2+i\eta)]-\ln^+[\xi-(2+i\eta)]\}=-\pi i.$$

With the help of this result we can find that ($\xi=2+it'$)

$$L_2^-\left[\frac{\xi}{2}\right]-L_2^+\left[\frac{\xi}{2}\right]=-\lim_{\eta\to+0}\tfrac{1}{2}\int_2^{2+it'}\{\ln^-[\lambda-(2+i\eta)]-\ln^+[\lambda-(2+i\eta)]\}\frac{1}{\lambda}\,d\lambda=\pi i\int_2^{2+it'}\frac{d\lambda}{\lambda}\cong-\frac{\pi}{2}t'\ .$$

This leads (small t') to

$$\frac{1}{\epsilon^{+}(\xi k_F)}-\frac{1}{\epsilon^{-}(\xi k_F)}\cong\pi D t' , \tag{35}$$

where D is given by (6) for free electrons and by (8) for zero-gap semiconductors. Inserting (35) into (33) and performing the integration we can find with the help of (32) function $A(t)$. Integral (31) can be evaluated with $H_0^{(1)}$ replaced by its asymptotic form since $k_F\zeta \gg 1$.

Asymptotic form of the potential $V(\zeta)$ when $k_F\zeta \gg 1$ is obtained by adding the nonoscillatory term V_n [Eq. (30)] to V_0 [Eq. (31)]. The result is [see Eqs. (6) or (8) for D]

$$V(\zeta)\cong\frac{2Q_{\text{ext}}k_F}{(k_F\zeta)^3}\left[\left[\frac{a(q_\parallel,0)}{q_\parallel/k_F}\right]^2_{q_\parallel=0}+\frac{D}{[1+a(2k_F,0)]^2}\cos(2k_F\zeta)\right] . \tag{36}$$

The rederived result here for free electrons is eight times less than that in Ref. 18.

As can be seen from Figs. 3–5, Friedel oscillations of $V(\zeta)$ are well pronounced in CdS and almost invisible in InSb and HgTe. The ratios of the amplitude of Friedel oscillations to the nonoscillatory term are 0.89, 0.03, and 0.05 for CdS, InSb, and HgTe, respectively, when electron concentration $n=10^{17}$ cm^{-3}. In HgTe the ratio of the potential given by (36) to the result of computer calculations rises from 8% at $\zeta=10^3$ a.u. to 66% at $\zeta=2.3\times10^3$ a.u.

Along with certain similarities in a long-range behavior of $V(\zeta)$ in semi-infinite InSb and HgTe, an essential difference appears in a short-range behavior of $V(\zeta)$ in these materials. In contrast to InSb, in HgTe large differences between $eV(\zeta)$ and the classical result $2e^2/(\epsilon_0+1)\zeta$ can still be observed when $k_F\zeta$ is of the order 10 a.u. (cf. Fig. 5). This is due to the logarithmic term in $V(\zeta)$ which appears in the case of semi-infinite gapless semiconductors only.

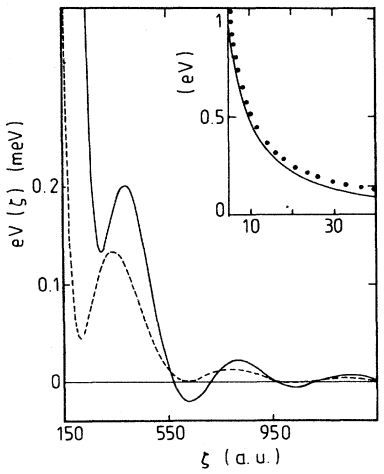

FIG. 3. Long- and short-range behavior of the potential along the surface, when the external point charge is on this surface for CdS when $n=10^{17}$ cm^{-3}. Solid lines, computer calculations according to Eq. (29). Dashed line, asymptotic form (36). Dotted line, the results for classical dielectric.

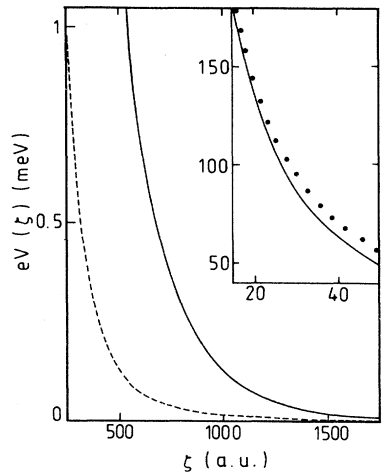

FIG. 4. Long- and short-range behavior of the potential along the surface, when the external point charge is on this surface for InSb when $n=10^{17}$ cm^{-3} ($\epsilon_0=18$, $m_e=0.02m_0$). Solid lines, computer calculations according to Eq. (29). Dashed line, asymptotic form (36). Dotted line, the results for classical dielectric.

E. Screening of a uniform electric field

We wish to calculate the screened potential $W(z)$ of the field $\mathbf{E}(z)$ which outside the semi-infinite semiconductor is $(0,0,E_0)$. It is convenient to assume that $\mathbf{E}(z)$ is

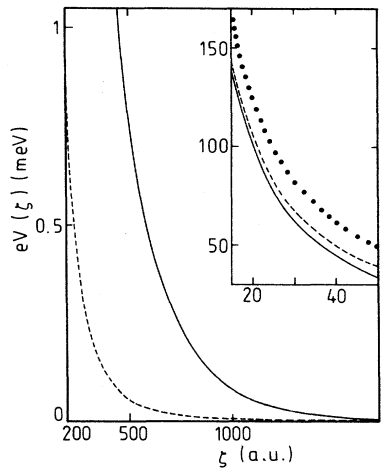

FIG. 5. Long- and short-range behavior of the potential along the surface when the external point charge is on this surface for HgTe when $n=10^{17}$ cm^{-3}. Dashed lines correspond to the asymptotic forms: (27) (with e^2/ζ added; $z=z_0=0$) for small ζ and (36) for large ζ, respectively. Solid lines, computer calculations according to Eq. (29). Dotted line the results for the classical dielectric.

produced by uniformly charged plate ($\omega=-E_0/4\pi$) parallel to the semiconductor surface and located at $z_0\to+\infty$. Now $W(z)$ for $z\le 0$ can be deduced from (11) and (12) by employing the superposition rule which gives

$$W(z)=\int_0^\infty d(k_F\zeta)k_F\zeta V(\zeta,z,z_0;Q_{\rm ext}=-E_0/2k_F^2)\ , \tag{37}$$

where V is the potential for $z\le 0$ due to the point charge $Q_{\rm ext}=-E_0/2k_F^2$ located at $z_0>0$. Thanks to the definition of Hankel transform: $F(t)=\int_0^\infty sf(s)J_0(st)ds$, $f(s)=\int_0^\infty tF(t)J_0(st)dt$, $W(z)$ given by (37) can be interpreted as a Hankel transform of V when $q_\parallel=0$, i.e., [see Eqs. (11) and (12)]

$$W(z)=\lim_{q_\parallel\to 0} v_s(q_\parallel,z,z_0)k_F^2/2\pi$$
$$=-\frac{E_0}{k_F}\left[\frac{a(q_\parallel,z)}{q_\parallel/k_F}\right]_{q_\parallel=0}\ . \tag{38}$$

From (13) we get (see, for example, Ref. 7)

$$W(z)=-\frac{2}{\pi}\frac{E_0}{k_F}\int_0^\infty d\xi\frac{\cos\xi z}{\xi^2\epsilon(\xi k_F)}$$
$$+\frac{2}{\pi}\frac{E_0}{k_F}\int_0^\infty\frac{d\xi}{\xi^2\epsilon(\xi k_F)}\ , \tag{39}$$

where the second term is a constant equal to $+(E_0/k_F)[a(q_\parallel,0)/(q_\parallel/k_F)]_{q_\parallel=0}$ and introduced in order to normalize $W(z)$ in such a way that $W(0)=0$.

The asymptotic form of $W(z)$ for large $|k_Fz|$ can be found with the help of the Lighthill method.[28] Deep inside the semiconductor, when $k_Fz\to\infty$, $W(z)$ takes the form

$$W(z)\cong\frac{E_0}{k_F}\frac{D}{2}\frac{\sin(2k_F|z|)}{(k_Fz)^2}+\frac{2}{\pi}\frac{E_0}{k_F}\int_0^\infty\frac{d\xi}{\xi^2\epsilon(\xi k_F)}\ , \tag{40}$$

where D is given by (6) and (8) for free electrons and for zero-gap semiconductors, respectively.

IV. SUMMARIES

We studied the influence of the electronic band structure of a zero-gap semiconductor on the asymptotic forms of the screened electrostatic potentials in both bulk and semi-infinite medium. Special emphasis was laid on Friedel oscillations which are considerably weaker in gapless materials compared to those in open-gap semiconductors, where the conduction-band carriers can be represented approximately by a free-electron gas. For example, in HgTe when the electron concentration n is 10^{17} cm^{-3} the amplitudes of the Friedel oscillations in the case of the screened Coulomb potential in the bulk are 41% less than those predicted by the theory for free electrons. One gets the same result for the screened uniform electric field in a semi-infinite medium.

When an external point charge is located at the surface of the gapless semiconductor, then at large distances along this surface the oscillatory part of the effective potential is very small compared to the nonoscillatory term (approximately 20 times less in the case of HgTe when $n=10^{17}$ cm^{-3}). The shape of the potential on a surface is of great importance when calculating the interaction of adatoms[15–19] and the heat of adsorption.[15]

We investigated also the form of the induced potential along z axis (normal to the semiconductor surface) when an external charge $Q_{\rm ext}$ is located at $\zeta=0,z_0$. The curve $V_{\rm ind}$ versus z lies between that of a classical dielectric and that of a classical metal. It turns out that the induced potential at the site of the external point charge [it is $V_{\rm ind}(\zeta=0,z,z_0=z)$] tends to $Q_{\rm ext}[(\epsilon_0-1)/(\epsilon_0+1)](2z)^{-1}$ (i.e., to the result for classical dielectric) ad $k_Fz\to 0+$. This means that in the case mentioned above free carriers in a semiconductor do not play a significant role in the process of screening near the surface (see, for example, Refs. 29–33 for comparison with the situation in the intrinsic semiconductors). The form of $V_{\rm ind}$ $(\zeta=0,z,z_0=z)/2$ (image-force potential) close to the surface plays an important role, for instance, in the description of the tunneling of electrons through the surface barrier in the field emission experiments.

An interesting consequence of the specific band structure of the gapless semiconductors is that in the presence of a surface $V_{\rm ind}(\zeta,z,z_0)$ contains an additional part of logarithmic type which diverges when $\zeta^2+(z+z_0)^2\to 0$ and which does not appear in the free-electron-gas case.

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