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Ionized-impurity scattering in the strong-screening limit

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We have developed a self-consistent multi-ion screening formalism which, unlike conventional treatments, explicitly assures that no electron state should contribute more than $-e$ to the net charge screening the donors. A key finding is that formal consistency can be achieved only when neighboring ion potentials overlap somewhat. Ionized-impurity scattering in a semiconductor is therefore intrinsically a multi-ion process, and the tightly screened, isolated-impurity regime is unphysical. Temperature- and doping-dependent majority-carrier mobilities for uncompensated n-type Si, Ge, GaAs, and InP are recalculated using the "multi-ion" screening length. The correction to the mobility is often substantial (as much as a factor of 4), and in some regimes the agreement between theory and experiment is considerably improved.

I. INTRODUCTION

Virtually all previous treatments of impurity screening by a free-electron gas in a doped semiconductor have been based on a linear extrapolation from the single-ion problem.[1,2] However, it will be shown in the following sections that the electrons are never able to screen a given ion in a multi-ion system as well as they can screen the same ion in a single-ion system. A self-consistent screening formalism will be developed which for the first time explicitly accounts for the fact that no electron can contribute more than one unit charge ($-e$) to the total screening of all donors. The qualitative differences between single-ion and multi-ion screening are particularly important in the "strong-screening" regime, where the screening length calculated by conventional methods is so short that neighboring impurity potentials do not overlap significantly.

The derived formalism is based on a breakdown of the free-electron screening charge in a way which is not usually considered, namely as a function of energy. Using the linearized Thomas-Fermi (LTF) approximation, one may calculate to reasonable accuracy the total electron charge density $\rho(\mathbf{r})$ devoted to the screening of a single donor. However, the LTF approach yields no information concerning how electrons with different energies contribute to $\rho(\mathbf{r})$. In an effort to obtain the energy dependence of the screening charge, it is tempting to use the expression for the generalized Friedel sum rule[3,4]

$$Z_I=\frac{2}{\pi k_B T}\int_0^\infty d\varepsilon f_0(1-f_0)\sum_{l=0}^{\infty}(2l+1)\delta_l(\varepsilon) \qquad (1.1)$$

which, in the single-ion limit, assures that a given impurity is "fully screened" at large distances. Here $Z_I e$ is the charge on the impurity, f_0 is the Fermi distribution function, and δ_l is the phase shift for the lth partial wave. The functional form of this integral would seem to imply that for degenerate statistics, only electrons with energies near the Fermi level contribute to the screening. However, it will be shown below that this argument is quite misleading.

In Sec. II we employ the Kohn-Sham formalism to obtain a reliable lowest-order expression for the energy dependence of the screening charge [and show that the charge represented by the right side of Eq. (1.1) is a physically distinct entity from the "screening charge"]. In Sec. III the energy-dependent expression is used to demonstrate that the conventional linear extrapolation from the single-ion case leads to a formal inconsistency. An improved formalism is then derived which removes this difficulty. Finally, in Sec. IV the "multi-ion screening length" is used to calculate revised electron mobilities. Detailed comparisons are made with experimental results for Si, Ge, GaAs, and InP as a function of doping level and temperature.

II. ENERGY DEPENDENCE OF THE SCREENING CHARGE

We consider a large sphere of radius R, which is filled with an electron gas of density n and a uniform background of positive charge with the same density. The medium has a static dielectric constant κ_0, and the electrons are characterized by an isotropic, parabolic effective mass m_e. This system is then perturbed by adding a point impurity charge $Z_I e$ at the center of the sphere as well as Z_I additional electrons to preserve charge neutrality. The Kohn-Sham density-functional formalism[5,6] yields that the excess electron charge density $\rho(\mathbf{r})$ may be found from the simultaneous solution of Poisson's equation

$$\nabla^2\phi(\mathbf{r})=\frac{4\pi e}{\kappa_0}\rho(\mathbf{r}) \qquad (2.1)$$

and the radial Schrödinger equations

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$$\left[-\frac{\hbar^2}{2m_e r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{l(l+1)\hbar^2}{2m_e r^2}+\phi(r)+\phi_{\mathrm{xc}}(r)\right]R_l=\frac{\hbar^2k_{nl}^2}{2m_e}R_l\ , \tag{2.2}$$

where $\phi(r)$ is the spherically symmetric screened electrostatic potential, $\phi_{\mathrm{xc}}(r)$ is the exchange-correlation potential, $R_l(k_{nl}r)$ is the radial wave function, and k_{nl} is the wave vector associated with the state having quantum numbers n and l. The excess charge density associated with screening may be written as the difference between the perturbed and unperturbed electron charges

$$\begin{aligned}\rho(r)&=-e\sum_{n,l,m,s}[\Psi^*_{nlms}\Psi_{nlms}f_0(\varepsilon_{nl})-\Psi^{0*}_{nlms}\Psi^0_{nlms}f_0(\varepsilon^0_{nl})]\\&=-2e\sum_n\sum_l(2l+1)\left[N_{nl}^2\frac{R_l^2(k_{nl}r)}{(k_{nl}r)^2}f_0(\varepsilon_{nl})-(N^0_{nl})^2j_l^2(k^0_{nl}r)f_0(\varepsilon^0_{nl})\right]\ .\end{aligned} \tag{2.3}$$

Here the j_l are spherical Bessel functions of the first kind and N_{nl} is the wave-function-normalization factor

$$N_{nl}^2 4\pi\int_0^R r^2\left[\frac{R_l(k_{nl}r)}{k_{nl}r}\right]^2 dr=1\ . \tag{2.4}$$

The large-r boundary condition of Eq. (2.2) is $R_l(k_{nl}R=X_{nl})=0$, where X_{nl} is the nth zero of R_l. From the asymptotic form

$$k^0_{nl}j_l(k^0_{nl}r)\rightarrow\sin(k^0_{nl}r-\tfrac{1}{2}l\pi) \tag{2.5}$$

we see that the unperturbed solution $R_l^0=(k^0_{nl}r)j_l(k^0_{nl}r)$ satisfies the boundary condition when $k^0_{nl}R=(n+\frac{1}{2}l)\pi$. Similarly, the phase-shifted asymptotic form of the perturbed solution

$$R_l(k_{nl}r)\rightarrow\sin(k_{nl}r-\tfrac{1}{2}l\pi+\delta_l) \tag{2.6}$$

gives $k_{nl}R=(n+\frac{1}{2}l)\pi-\delta_l$. We have specifically defined R_l such that at large r the amplitudes of the oscillating perturbed and unperturbed wave functions are the same, with any further multiplicative constants being absorbed into the normalization factor N_{nl}. The other boundary conditions are

$$R_l(r\rightarrow 0)\rightarrow 0,\quad \phi(r\rightarrow 0)\rightarrow -Z_Ie^2/\kappa_0 r\ ,$$

and

$$\phi(r\geq a)\rightarrow 0\ ,$$

where $a \ll R$ is a radius on the order of a few screening lengths beyond which the ion potential may be ignored.

The bracketed expression of Eq. (2.3) contains three factors which are different for the perturbed and unperturbed systems. It will be seen below that corrections due to any two of the three factors are never large at the same time. It is therefore valid to decompose the excess charge density into three parts $\rho(r)=\rho_1(r)+\rho_2(r)+\rho_3(r)$, corresponding to a "normalization-correction" term

$$\rho_1(r)=-2e\sum_n\sum_l(2l+1)[N_{nl}^2-(N^0_{nl})^2]\ j_l^2(k^0_{nl}r)f_0(\varepsilon^0_{nl}) \tag{2.7}$$

a "density-of-states" term

$$\begin{aligned}\rho_2(r)&=-2e\sum_n\sum_l(2l+1)(N^0_{nl})^2j_l^2(k^0_{nl}r)[f_0(\varepsilon_{nl})-f_0(\varepsilon^0_{nl})]\\&\approx-4e\sum_n\sum_l(2l+1)(N^0_{nl})^2j_l^2(k^0_{nl}r)f_0(\varepsilon^0_{nl})[1-f_0(\varepsilon^0_{nl})]\frac{\delta_l(k^0_{nl})\varepsilon^0_{nl}}{(k^0_{nl}R)k_BT}\end{aligned} \tag{2.8}$$

and a "wave-function-redistribution" term

$$\rho_3(r)=-2e\sum_n\sum_l(2l+1)(N^0_{nl})^2\left[\frac{R_l^2(k_{nl}r)}{(k_{nl}r)^2}-j_l^2(k^0_{nl}r)\right]f_0(\varepsilon^0_{nl})\ , \tag{2.9}$$

where $f_0(\varepsilon_{nl})$ in Eq. (2.8) has been expanded in a Taylor series about ε^0_{nl}. We also define the integrated charge associated with each term

$$P_j=4\pi\int_0^R\rho_j(r)r^2dr \tag{2.10}$$

and the total charge $P=P_1+P_2+P_3$.

One finds that $\rho_3(r)$ is the only term which contributes appreciably within the small sphere $r<a$. This is because P_1 and P_2 are distributed relatively uniformly[7] within the much larger sphere $r<R$. Because the impurity charge Z_Ie must be completely screened within $r<a$, the integral of $\rho_3(r)$ in this region must yield $-Z_Ie$. For $r>a$ we can use the large-r forms of the perturbed and unperturbed wave functions [Eqs. (2.5) and (2.6)] in Eq. (2.9) to find that $\rho_3(r>a)\approx 0$. Thus $P_3=-Z_Ie$. Furthermore, P_1+P_3 must vanish identically since these two terms represent only a spatial redistribution of charge within the same set of electron states. We therefore find that $P_1 = Z_I e$ and that $P = P_2$. Recalling that Z_I electrons were added to the perturbed system, it follows that $P_2 = -Z_I e$. While only ρ_3 is important in the region $r < a$, both ρ_1 and ρ_2 contribute when $r > a$. They cancel, however, leaving the charge density far away from the impurity essentially the same as in the unperturbed case.

The generalized Friedel sum rule may be derived by writing $Z_I = -P_2/e$, and performing the integral in Eq. (2.10) using the normalization condition [Eq. (2.4)]. Converting the sum over n to an integral over energy

$$\left[(2\pi/R)\sum_n \to (2m_e/\hbar^2\varepsilon)^{1/2}d\varepsilon\right]$$

then leads immediately to Eq. (1.1). As was mentioned in the Introduction, the additional charge added to the system in order to preserve charge neutrality (ρ_2) is equal in magnitude but physically distinct from the actual "screening charge" (ρ_3) located in the immediate vicinity of the impurity. It is therefore ρ_3 rather than ρ_2 which must now be examined in order to determine the energy distribution of electrons screening the impurity.

Having shown that ρ_1 and ρ_2 are unimportant when $r < a$, we consider $\rho(r) \approx \rho_3(r)$ in that region. Converting the sum over n to an integral and using the relation $(N_{nl}^0)^2 = m_e\varepsilon/\pi\hbar^2 R$, Eq. (2.9) becomes

$$\rho(r<a) = -\frac{e}{2\pi^2}\left[\frac{2m_e}{\hbar^2}\right]^{3/2} \times \int_0^\infty d\varepsilon\, f_0(\varepsilon)\varepsilon^{1/2} \times \sum_{l=0}^{\infty}(2l+1)\left[\frac{R_l^2(kr)}{(kr)^2} - j_l^2(kr)\right] . \tag{2.11}$$

In general, the simultaneous equations (2.1), (2.2), and (2.11) must be solved numerically.[8,9] However, it is shown in the Appendix that the summation over l may be evaluated in the limit of weak potentials, where the LTF approximation is valid. Ignoring the exchange-correlation contribution to the effective potential,[10] we obtain

$$\rho(r) \approx \frac{e\phi(r)}{4\pi^2}\left[\frac{2m_e}{\hbar^2}\right]^{3/2}\int_0^\infty \frac{f_0 d\varepsilon}{\varepsilon^{1/2}} . \tag{2.12}$$

This is the desired result which gives the contribution to the screening by electrons as a function of energy. It is easily verified that when the integral in Eq. (2.12) is evaluated, one obtains the conventional LTF result

$$\rho_{\text{LTF}}(r) = \frac{neF'(\eta)\phi(r)}{k_B T} , \tag{2.13}$$

where n is the total electron density, $\eta \equiv \varepsilon_F/k_B T$ is the reduced Fermi energy,

$$F'(\eta) \equiv \frac{\mathcal{F}_{-1/2}(\eta)}{\mathcal{F}_{1/2}(\eta)} \tag{2.14}$$

and the $\mathcal{F}_p$ are Fermi integrals.[11] However, rather than performing the integral, we instead use Eq. (2.12) to determine the charge density contributed by a single electron in state i with energy ε. We write[12]

$$\rho(r) = \sum_i \bar{\rho}_i(r) f_0(\varepsilon_i) \tag{2.15}$$

which implies[13]

$$\bar{\rho}_i(r) = -e[\,|\Psi_i(r)|^2 - |\Psi_i^0(r)|^2] \approx \frac{e\phi(r)}{2V\varepsilon_i} . \tag{2.16}$$

Here $V = 4\pi R^3/3$ is the total volume of the system and we have used the operator relation

$$\sum_i \to \frac{V}{2\pi^2}\left[\frac{2m_e}{\hbar^2}\right]^{3/2}\int_0^\infty \varepsilon^{1/2} d\varepsilon . \tag{2.17}$$

If the potential $\phi(r)$ appearing in Eq. (2.16) is evaluated by substituting the LTF charge density [Eq. (2.13)] into Poisson's equation [(2.1)], one obtains a simple screened Coulomb potential[1,2]

$$\phi(r) = -\frac{e^2 e^{-r/\lambda}}{\kappa_0 r} , \tag{2.18}$$

where λ is the screening length and for simplicity we assume $Z_I = 1$. In this approximation, λ is given by[1]

$$\lambda_0^{-2} = \frac{4\pi n e^2 F'(\eta)}{\kappa_0 k_B T} . \tag{2.19}$$

Combining Eqs. (2.16) and (2.18), one finds that the total screening charge contributed by state i to the screening of a single impurity (called j) is given by

$$q_{ij} = \int d^3r\, \bar{\rho}_i(\mathbf{r}) \to -\frac{2\pi e^3\lambda^2}{V\kappa_0\varepsilon_i} . \tag{2.20}$$

This simple, first-order result shows that in the single-ion problem, low-energy electrons contribute much more to the screening than do high-energy electrons. This should not be surprising, since it is well known that low-energy electrons have much stronger interactions with ionized impurities. However, q_{ij} is always much less than the total electron charge $-e$ because the system volume V can be made arbitrarily large.

III. MULTI-ION SCREENING

In this section we demonstrate that even though LTF provides a useful lowest-order approximation for the screened single-ion scattering potential, generalization to the multi-ion problem by the usual procedure leads to physically unreasonable results. This is most easily understood if we first consider the "strong-screening" regime, where the LTF screening length λ_0 is much shorter than the average distance between impurities and where neighboring ion potentials do not overlap significantly. However, the final results will be in a form which applies to any uncompensated semiconductor.

In the LTF approximation, the net multi-ion potential is simply a linear superposition of single-ion potentials

$$\phi_T(\mathbf{r}) = -\sum_{j=1}^{\mathcal{N}_D} \frac{e^2 e^{-|\mathbf{r}-\mathbf{r}_j|/\lambda}}{\kappa_0|\mathbf{r}-\mathbf{r}_j|} , \tag{3.1}$$

where $\mathbf{r}_j$ is the position of the jth donor and $\mathcal{N}_D$ is the total number of donors in the system. Using Eqs. (2.20) and (2.16), one finds that the net charge contributed by a given electron to the screening of all donors is

$$Q_i = \sum_{j=1}^{\mathcal{N}_D} q_{ij} \to -\frac{2\pi N_D e^3 \lambda^2}{\kappa_0 \varepsilon_i} . \tag{3.2}$$

Here $N_D = \mathcal{N}_D / V$ is the donor density, which is equal to n when there is no compensation.

If Q_i is summed over electron states, one finds that in LTF the total screening charge exactly neutralizes the donor charges

$$\sum_i -\frac{Q_i}{e} f_0(\varepsilon_i) = \mathcal{N}_D . \tag{3.3}$$

However, a closer examination of Eq. (3.2) shows that this procedure contains an inconsistency. For high-energy electrons $-Q_i/e < 1$, that is, a given electron's total charge $-e$ is not completely devoted to screening. On the other hand, evaluation of Eq. (3.2) for low-energy electrons leads to the relation $-Q_i/e > 1$, indicating that the assumed contribution to the screening is greater than the charge available. This is physically unreasonable since we are specifically considering the regime where LTF theory predicts no significant overlap of neighboring donor potentials (a given quantity of electron charge cannot simultaneously contribute to the screening of more than one donor).

In a more realistic calculation of the screening, we must require that $-Q_i/e \leq 1$ for all electrons. The simplest way of accomplishing this is to multiply the charge density for state i in Eq. (2.16) by an additional factor S_i

$$\bar{\rho}_i'(\mathbf{r}) \to S_i \bar{\rho}_i(\mathbf{r}) , \tag{3.4}$$

where

$$\begin{aligned} S_i(\varepsilon_i) &= \frac{\mathcal{E}}{\varepsilon_i}, \quad \varepsilon_i < \mathcal{E} \\ &= 1, \quad \varepsilon_i \geq \mathcal{E} \end{aligned} \tag{3.5}$$

and

$$\mathcal{E} = \varepsilon_q' \equiv \frac{2\pi N_D e^2 \lambda^2}{\kappa_0} . \tag{3.6}$$

Using Eqs. (2.20) and (3.2), one immediately obtains for the corrected screening charge $Q_i' = S_i Q_i$.

Since $-Q_i/e$ for low-energy electrons has been effectively decreased (it may no longer exceed unity) Eq. (3.3) no longer holds. While each low-energy electron ($\varepsilon_i < \varepsilon_q'$) now contributes a charge of exactly $-e$ to the screening of the donors, the high-energy electrons ($\varepsilon_i > \varepsilon_q'$) do not screen effectively and each contributes less than its total charge.[14] Since $n = N_D$, this implies that the donors are not fully screened. Varying the screening length from λ_0 to some λ' does not remove the apparent difficulty because no matter how much the screening length (and hence ε_q') is increased, there are always electrons in the high-energy tail of the finite-temperature Fermi distribution which are not fully devoted to screening. We conclude that Eq. (3.3) can never be satisfied. However, this is not a drawback as long as neighboring potentials overlap somewhat. At distances greater than half the average interdonor separation, $D = (4\pi N_D/3)^{-1/3}$, it is unnecessary to insist that each donor be fully screened, only that overall charge neutrality be preserved.[15] This considerably relaxes the magnitude of the total screening charge required and makes it unnecessary to satisfy Eq. (3.3).

Although we do not require that each donor be fully screened independently of the others, there must still be enough electron charge available to provide screening out to the overlap region. "Complete" screening of a given donor would require that the excess electron charge integrated over all space add up to exactly $-e$. Here we define g to be that fraction of the total which would be contained within a sphere of radius D surrounding the donor. Using the proportionality of $\rho(\mathbf{r})$ to $\phi(\mathbf{r})$, we have

$$\begin{aligned} g &= \frac{4\pi \int_0^D \phi(r) r^2 dr}{4\pi \int_0^\infty \phi(r) r^2 dr} \\ &\to 1 - \left[1 + \frac{D}{\lambda_M} \right] e^{-D/\lambda_M} , \end{aligned} \tag{3.7}$$

where the "multi-ion" screening length λ_M will be defined below. We now rewrite Eq. (3.3) to reflect the relaxed requirement that the total donor charge to be screened has been reduced by a factor of g

$$\sum_i -\frac{Q_i''}{e} f_0(\varepsilon_i) = g \mathcal{N}_D . \tag{3.8}$$

The restricted region of integration also causes the electron charge per donor q_{ij} to be smaller by the same factor. Using Eqs. (2.20), (3.2), and (3.4), the total screening charge for a given state i becomes

$$Q_i'' = -\frac{2\pi g N_D e^3 \lambda^2 S_i}{\kappa_0 \varepsilon_i} . \tag{3.9}$$

Again, we must not allow this charge to exceed $-e$. In Eq. (3.5) for S_i, we therefore set

$$\mathcal{E} = \varepsilon_q'' \equiv \frac{2\pi g N_D e^2 \lambda_M^2}{\kappa_0} . \tag{3.10}$$

The screening-charge requirements may now be fulfilled by adjusting the screening length λ_M until Eq. (3.8) is satisfied. This condition may be written in the compact form

$$\lambda_M^{-2} = \Gamma \lambda_0^{-2} , \tag{3.11}$$

where

$$\Gamma = \frac{\int_0^{z_q} \frac{z^{1/2}}{z_q} f_0 dz + \int_{z_q}^\infty z^{-1/2} f_0 dz}{\int_0^\infty z^{-1/2} f_0 dz} \tag{3.12}$$

and

$$z_q \equiv \frac{\varepsilon_q''}{k_B T} = \frac{2\pi g N_D e^2 \lambda_M^2}{\kappa_0 k_B T} . \tag{3.13}$$

We refer to λ_M as the "multi-ion" screening length because its value is quite sensitive to the interdonor spacing (through the factor g).

An interesting implication of the preceding analysis is that the "strong-screening" limit, in which each impurity potential may be considered well isolated from its neighbors, is found to be unphysical. This is because Eq. (3.8) can never be satisfied unless neighboring impurity potentials have at least a modest amount of overlap. We conclude that ionized-impurity scattering in a semiconductor is intrinsically a multi-ion process.

IV. ELECTRON TRANSPORT AND COMPARISON WITH EXPERIMENT

In the previous section, it was shown that the screening length in a multi-ion system must always exceed the value predicted by conventional single-ion calculations. The results of that analysis will now be used to assess the importance of multi-ion screening in semiconductor free-carrier transport. To illustrate, we calculate electron mobilities as a function of donor density and temperature for uncompensated silicon, germanium, GaAs, and InP.

Naturally, the importance of the multi-ion screening correction depends both on the amount by which λ_M exceeds λ_0 and on the sensitivity of the scattering to variations in the screening length. In discussing the former, it is useful to rewrite Eq. (3.13) as

$$\frac{z_q}{z_0} = \frac{g}{3\Gamma} \left[\frac{N_D}{n} \right] , \tag{4.1}$$

where $z_0 = 3/2F'(\eta)$ is the average electron energy. From Eq. (3.12), it is evident that the multi-ion screening correction is largest when z_q/z_0 is large. This favors either high compensation (since the greater N_D/n, the more difficult it is for a given number of electrons to screen all donors simultaneously[16]) or large g (the strong-screening regime[17]). However in the specific calculations which follow the screening correction for uncompensated materials tends to lie within the fairly narrow range $1.07 < \lambda_M/\lambda_0 < 1.45$. Thus the more significant consideration is the sensitivity of the mobility to changes in the screening length. From a lowest-order Brooks-Herring calculation,[18] one finds that the momentum-transfer scattering cross section depends on λ through the factor

$$g' = \ln(b+1) - \frac{b}{b+1} , \tag{4.2}$$

where $b \equiv 4k^2\lambda^2$. Evaluation at a wave vector corresponding to the "average" electron energy yields

$$b \approx \frac{9.3}{F'^{\,2}\Gamma} \left[\frac{\kappa_0}{16} \right] \left[\frac{m_{\rm ds}}{m_0} \right] \left[\frac{n}{10^{19}} \right]^{-1} \left[\frac{T}{300} \right]^2 , \tag{4.3}$$

where $m_{\rm dc}$ is the density-of-states effective mass. When b is large (low densities or high temperatures), the scattering cross section has only a logarithmic dependence on λ and the multi-ion screening correction will have negligible effect on the transport properties. However, in the small-b limit one has $g' \propto b^2 \propto \lambda^4$, and any increase of λ by 1.19 or more leads to at least a factor of 2 decrease in the mobility. Multi-ion screening effects are therefore far more important in the strong-screening regime where b is small. One should note that despite the n^{-1} factor, b for a given material at a given temperature does not decrease monotonically with increasing carrier density. As soon as the carrier population starts to become degenerate ($\eta > 0$), the factor $(F')^{-2}$ causes b to increase with further increases in n. The very smallest values of b and hence the highest sensitivity to multi-ion screening would probably be observed for minority transport of a carrier with light effective mass in a heavily doped material. In that case a very short screening length would be combined with a very small wave vector.

In obtaining the electron mobilities to be discussed below, we have employed the multi-ion screening length λ_M rather than the conventional single-site result λ_0. However, the single-site scattering picture[19] has then been used to obtain transition rates based on the altered ion potentials. In contrast to most previous calculations, momentum-transfer scattering cross sections have been calculated by the partial-wave phase-shift method[20,21] instead of Brooks-Herring theory,[18] in order to avoid errors introduced by the Born approximation. In combining the multi-ion screening correction with the phase-shift method it is necessary to modify the generalized Friedel sum rule[3,4,20] [Eq. (1.1)], since "complete" screening of each donor can no longer be required [see the discussion preceding Eq. (3.8)]. Because the sum rule should still be satisfied in the limit where the multi-ion screening correction is negligible (i.e., when $\Gamma \approx 1$), we replace Eq. (3.11) by

$$\lambda_M^{-2} = \Gamma \lambda_F^{-2} , \tag{4.4}$$

where λ_F is that screening length which satisfies the generalized Friedel sum rule[20] rather than the LTF value.

In the mobility calculation[22] we have solved the Boltzmann equation by Kohler's variational method,[23] which accurately accounts for an arbitrary number of elastic and inelastic scattering processes. Mechanisms considered include ionized-impurity scattering, electron-electron scattering, and acoustic-, piezoelectric-, nonpolar-optical-, and polar-optical-phonon scattering. For GaAs and InP, conduction-band nonparabolicity was incorporated into the formalism.[24] Theoretical drift mobilities have been multiplied by the Hall factor r_H in order to allow direct comparison with experimental Hall results.[25] For silicon and germanium, the anisotropy correction[26] to r_H has been included. Otherwise, anisotropy effects have been treated only by using different "conductivity" and "density-of-states" effective masses. Material parameters employed in the calculations were taken from Ref. 22 for silicon, Ref. 27 for germanium, Ref. 28 for GaAs, and Ref. 29 for InP. Phonon parameters for each material were adjusted slightly to assure agreement with experiment at high temperatures and low doping levels.

A. Silicon

Figure 1 gives theoretical and experimental electron mobilities for uncompensated Si:P in the low-temperature limit. Comparison of the solid curve (multi-ion screening) with the dashed curve (conventional screening) indicates that multi-ion effects are quite significant in this regime. The figure illustrates that the conventional calculation leads to mobilities which are too high by as much as a factor of 4 near n_c, the critical density for the metal-insulator transition ($\approx 3.7\times10^{18}$ cm^{-3}). This is because b is small (on the order of 0.5), and the mobility is quite sensitive to changes in the screening length. The figure also shows that the agreement with experiment[30–32] is much better when the more consistent treatment of the screening is employed, although it should be remembered that there are additional higher-order effects which can lead to theoretical uncertainties.[33] For example, Krieger *et al.*[32,34] have suggested that the large discrepancy between the conventional theory and experiment may be due to the effect of conduction-band anisotropy on the screening. However, the more recent results of Saso and Kasuya for germanium,[9] which has an electron effective mass even more anisotropic than that of silicon, seem to indicate that screening anisotropy has a relatively small effect on the calculated mobility. The theoretical curves in Fig. 1 do not reproduce the precipitous drop of the mobility as n_c is approached from above, since we have made no attempt to include localization or impurity-banding effects in the free-electron calculation.

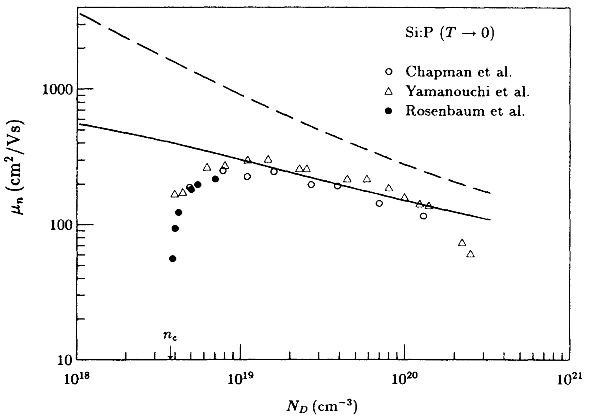

FIG. 1. Hall mobilities for uncompensated n-type Si:P extrapolated to the low-temperature limit. Experimental points (Refs. 30–32) are compared with the conventional screening theory (dashed curve) and the multi-ion screening theory (solid curve). The critical density n_c for the metal-insulator transition is indicated.

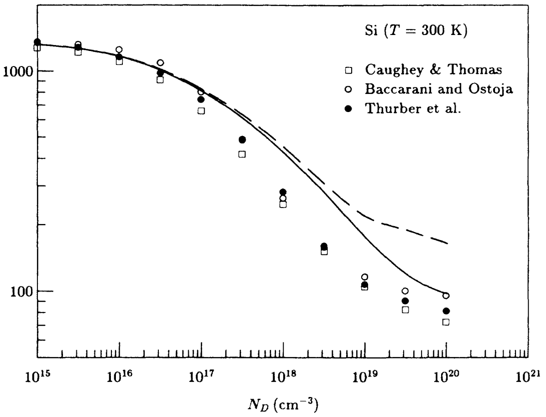

FIG. 2. Hall mobilities for uncompensated n-type Si:P at 300 K. Experimental points (Refs. 35–37) are compared with the conventional screening theory (dashed curve) and the multi-ion screening theory (solid curve).

Figure 2 shows a similar plot for uncompensated n-type silicon at 300 K. At this temperature the multi-ion screening correction has little effect when the doping level is below 10^{18} cm^{-3}, since b is large in that region (≥ 40). However, b decreases rapidly with increasing n, until at 10^{20} cm^{-3} it is only 1.7. Then the scattering becomes much more sensitive to changes in the screening length and the conventional calculation (dashed curve) introduces nearly a factor of 2 error in the mobility. The corrected mobilities (solid curve) are in considerably better agreement with experiment[35–37] at the highest densities.

However, even when the multi-ion screening correction is included the calculated mobilities are somewhat too high at intermediate doping levels. (At $N_D \approx 3\times10^{18}$ cm^{-3}, the discrepancy is a factor of 1.7. It would be 20% larger were Brooks-Herring theory employed rather than the phase-shift formalism.) The source of this disagreement is unclear, but it may be related either to the large effective-mass anisotropy of the conduction-band valleys[26] or to distortion of the free-electron wave functions and energies[39–40] by interactions with impurities, similar to those which lead to localization and the metal-insulator transition at low temperatures. (Factors such as partial freezeout of the electrons onto donor sites[41] and uncertainties in the precise doping levels[37] probably introduce only second-order errors.) Although Li and Thurber,[41] and Bennett[42] have claimed good agreement between their theories and experiment, the effects of electron-electron scattering were significantly overestimated in both of those studies. While they multiplied the ionized-impurity-scattering mobility by a constant factor[43] of 0.63, Appel[44] has shown that the correction should depend strongly on the value of the screening parameter b. He obtains 0.57 in the large-b limit, but greater than 0.95 when $b \leq 10$. Using Appel's scattering rates in conjunction with the Kohler variational method for solving the Boltzmann equation, we find that the electron-electron scattering correction for silicon at 300 K is never greater than a few percent at any doping level.[45] Tosic *et al.*,[39] also obtained good agreement with experiment using a calculation in which the electron density of states was altered by the presence of an impurity band. However, the impurity band is assumed to remain distinct up to the highest densities (with a constant donor binding energy). In a more realistic model the binding energy should decrease with doping level until it vanishes[46] above $n \approx 10^{19}$ cm^{-3}. Both Tosic *et al.* and Bennett employed a "conductivity" effective mass[47] which is considerably larger than the accepted value of 0.26. We conclude that while the inclusion of multi-ion screening improves the agreement between theory and experiment for *n*-type silicon at room temperature, there is presently no comprehensive theoretical treatment which accurately accounts for all of the data.

B. Germanium

Figure 3 shows calculated and experimental[48–55] electron mobilities for uncompensated germanium at low temperatures. The marked dependence of the experimental results on dopant (Sb or As) is thought to be due primarily to scattering by the stronger core potentials of the As impurity atoms.[56,57] Since core scattering is not included in our mobility formalism, it is probably more appropriate to compare the theoretical results with Sb-doped data.

For doping levels below 2×10^{18} cm^{-3}, the multi-ion screening calculation (solid curve) is in considerably better agreement with experiment than the conventional theory (dashed curve). Although the solid curve overcorrects by about 30% at higher densities when comparison is made with the Sb-doped data, this relatively small disagreement may be due to our approximate treatment of the large anisotropy of the electron effective mass. As they did for low-temperature silicon, Krieger and Meeks[58] have argued qualitatively that inclusion of mass anisotropy into the multivalley screening calculation leads to less-effective screening and hence lower mobilities than in the isotropic case. However, Saso and Kasuya[9] have performed a more detailed calculation of the random-phase-approximation (RPA) dielectric constant including mass anisotropy, and their results indicate a relatively modest correction to the mobility (about 20% at 10^{18} cm^{-3}). Saso and Kasuya have also performed a Kohn-Sham calculation of the phase shifts, which yielded a stronger scattering potential than the conventional LTF result. While their theoretical mobilities agreed well with experimental values at doping levels above 2×10^{18} cm^{-3}, they were too high by factors on the order of 2 at lower densities. The development of a Kohn-Sham calculation which includes the multi-ion screening effect (suggested in Ref. 19) should improve considerably the agreement of their calculation with the experimental results.[59]

Theoretical and experimental[47–50,59–62] results for germanium at room temperature are shown in Fig. 4. In this case, the agreement between theory and the Sb-doped data is quite good at all densities. Here the multi-ion screening correction never exceeds 30% since the lighter effective mass in germanium leads to increased degeneracy, which in turn prevents b from becoming as small as the minimum value noted above for silicon. It will be seen that in GaAs and InP, which have even smaller effective masses, the multi-ion screening correction to the room-temperature mobility is even less important ($\leq 10\%$). The previous calculation of Rode[27] gave mobilities for uncompensated germanium at 300 K which were somewhat higher than the experimental results, probably because of errors introduced by the use of Brooks-Herring theory and conventional rather than multi-ion screening (the combined correction is 40% at 10^{19} cm^{-3}).

C. GaAs

The most commonly used method for determining compensation densities in *n*-type GaAs has been to com-

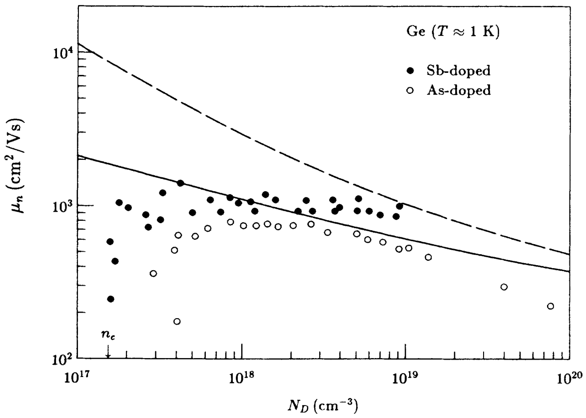

FIG. 3. Hall mobilities for uncompensated *n*-type Ge:Sb and Ge:As at $T \approx 1$ K. Experimental points (Refs. 48–55) are compared with the conventional screening theory (dashed curve) and the multi-ion screening theory (solid curve). The critical density n_c for the metal-insulator transition in Ge:Sb is indicated (it is slightly larger in Ge:As).

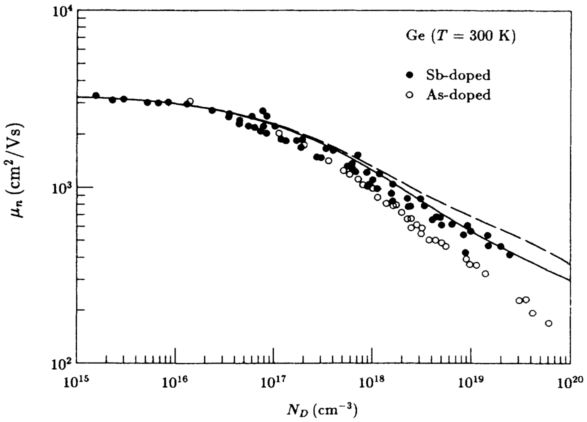

FIG. 4. Hall mobilities for uncompensated *n*-type Ge:Sb and Ge:As at 300 K. Experimental points (Refs. 48–51 and 60–63) are compared with the conventional screening theory (dashed curve) and the multi-ion screening theory (solid curve).

pare the measured electron mobility at an intermediate temperature (e.g., 77 K) with theory,[29,64,65] using N_A as an adjustable parameter. It has been widely noted[66,67] that this manner of characterization leads to acceptor concentrations which are never less than 30–50% of the donor densities, a finding that is relatively independent of the dopant and growth process. It has therefore been argued that GaAs is intrinsically self-compensating.[66] However, these conclusions depend heavily on the reliability of the calculated mobilities, and both of the models usually employed in the fitting[29,64,65] are based on Brooks-Herring theory.

Figure 5 shows theoretical and experimental[68–72] Hall mobilities for n-type GaAs at 77 K, where $N_A = 0$ has been assumed in the calculations. Note that when both the phase-shift correction to Brooks-Herring theory and the multi-ion screening correction are omitted (dashed curve), the calculation yields mobilities which are as much as 70% higher than the experimental values. Results such as these led previous investigators to conclude that around 35% compensation would be required to bring the two into agreement. However, the most general theory[73] (solid curve) is $\leq 25\%$ too high, which must be considered within the limits of theoretical uncertainties. Only $\approx 13\%$ compensation would be needed to achieve agreement.

When comparison is made to the more detailed theoretical treatment, we find that the mobility data at 77 K provide little evidence for significant self-compensation. This is in agreement with the conclusions of Poth *et al.*,[74] who argued that while the measured mobilities are not found to vary appreciably with donor species or growth parameters, the degree of self-compensation should. Kamiya and Wagner[75] also argued for minimal compensation in some of their samples, based on a technique using line-shape analysis of impurity photoluminescence spectra. Although Wolfe and Stillman[66] obtained an average compensation of 25% in lightly doped samples from a fit to the temperature dependence of the Hall coefficient R_H, those same authors[76] noted that the possible error in the analysis due to uncertainties in the treatment of excited impurity states is at least 17%. They also pointed out that the determination of N_A from $R_H(T)$ is unreliable at donor concentrations above $\approx 5\times 10^{15}$ cm^{-3}. Using free-carrier absorption measurements, Walukiewicz *et al.*[77] obtained significant compensation densities which appeared to agree well with mobility-analysis results on the same samples. However, both of their techniques relied on the accuracy of theoretical models for the ionized-impurity scattering rates.

Several authors[72,78–80] have employed detailed mobility analyses to investigate the apparent presence of an additional mechanism such as space-charge or central-cell scattering. Assuming that the unknown process has a mobility of the form $\mu_U = A_U T^{-1/2}$, both the acceptor density and A_U have been treated as adjustable parameters. However, since the additional scattering mechanism does not even dominate at most temperatures, this type of two-parameter fit is only meaningful if the "conventional" processes are unambiguously characterized. We have seen above that transport formalisms based on Brooks-Herring theory and single-ion screening yield GaAs mobilities which contain relatively large temperature-dependent errors. One must therefore question the reliability of even qualitative conclusions based on detailed analyses using such formalisms.

Figure 6 shows that at 300 K the assumption of uncompensated materials ($N_A = 0$) leads to excellent agreement between the most general theory (solid curve) and the data.[69–72,81] Mobilities calculated using conventional screening and Brooks-Herring theory (dashed curve) are only 15% higher, which is probably no larger than the theoretical uncertainty.[33] However, this difference is just large enough to cause the dashed curve to appear high when compared to the data. (See also Fig. 2 of Kuphal *et al.*[71])

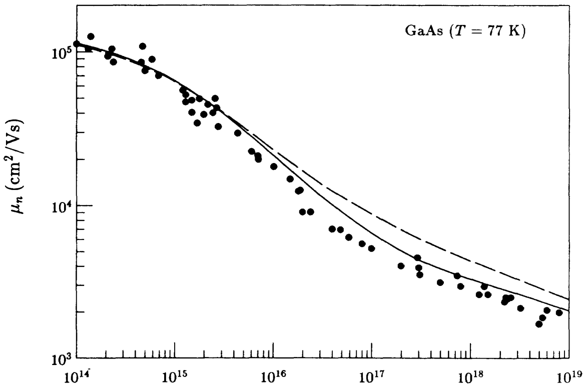

FIG. 5. Hall mobilities for uncompensated n-type GaAs at 77 K. Experimental points (Refs. 68–72) are compared to Brooks-Herring theory with conventional screening (dashed curve) and to the phase-shift formalism with multi-ion screening (solid curve).

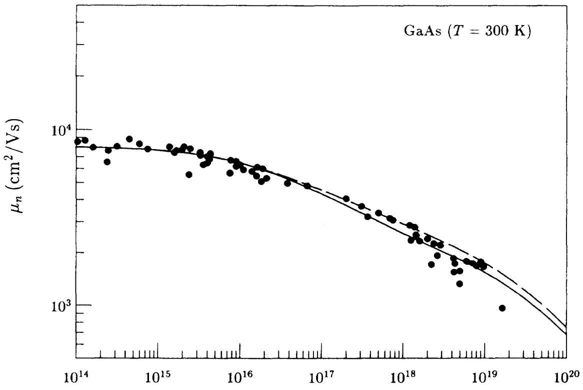

FIG. 6. Hall mobilities for uncompensated n-type GaAs at 300 K. Experimental points (Refs. 69–72 and 81) are compared to Brooks-Herring theory with conventional screening (dashed curve) and to the phase-shift formalism with multi-ion screening (solid curve).

D. InP

As in the case of GaAs, the highest mobilities reported for *n*-type InP at 77 K are seemingly independent of dopant.[82] Also similar is the finding[82–87] that the data can only be fit by conventional transport calculations[83–85] if at least 30–35 % self-compensation is assumed. This can be seen by comparing the dashed curve in Fig. 7 with the experimental points (the data from Anderson *et al.*[82] are consistent with other experimental results from the literature[85–87]). However, incorporation of the phase-shift and multi-ion screening corrections (solid curve) again reduces the maximum discrepancy to below 25%, corresponding to less than 13% compensation. Significantly, the solid and dashed curves begin to differ when $N_D \geq 10^{16}$ cm^{-3}, which is precisely the density above which a marked increase in the self-compensation is needed if the data are to be fit by the conventional theory.[82] Since no autocompensation is apparent from a chemical analysis of S-doped epitaxial layers,[82] Anderson *et al.* have attempted to improve the agreement with conventional theory by applying the lowest-order multi-ion scattering correction of Moore.[88] Although the correction factor of 2 is well outside the limits of validity claimed by Moore, the agreement between theory and experiment is improved in some regions. However, we have pointed out previously[89] that the next term in the multi-ion expansion is comparable to the lowest-order correction obtained by Moore and that any truncation of the expansion after a few terms may be invalid even when the low-order terms are small. The improved agreement resulting from the lowest-order multi-ion scattering correction must therefore be considered fortuitous.

Figure 8 shows the data[82] (points), conventional theory (dashed curve), and theory containing multi-ion screening and the phase-shift correction (solid curve) for *n*-type InP at 300 K. Although the more general theory marginally worsens the agreement with experiment at intermediate densities (the discrepancy is never more than 20%), it somewhat improves the agreement at high densities. As with GaAs, we find that multi-ion screening considerations do not have a large effect on the transport at 300 K.

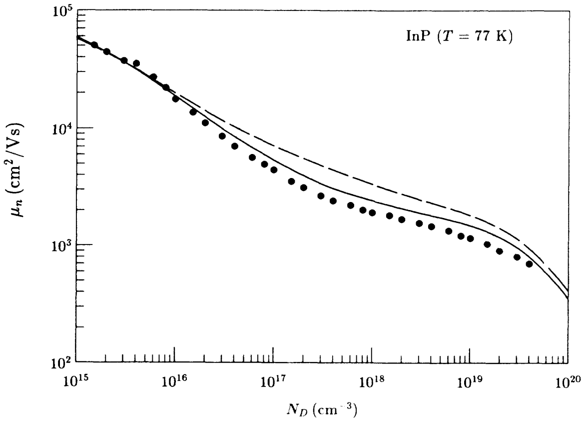

FIG. 7. Hall mobilities for uncompensated *n*-type InP at 77 K. Experimental points (Ref. 82) are compared to Brooks-Herring theory with conventional screening (dashed curve) and to the phase-shift formalism with multi-ion screening (solid curve).

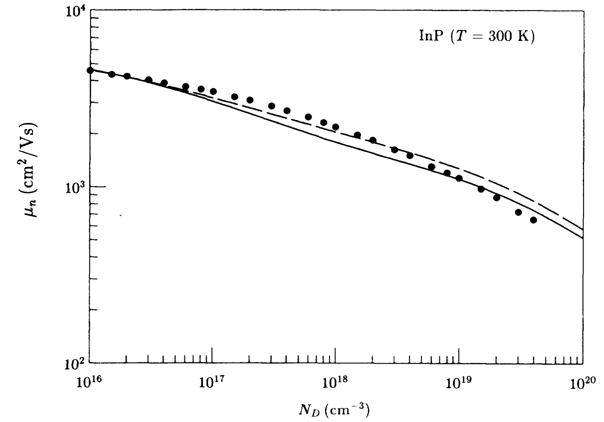

FIG. 8. Hall mobilities for uncompensated *n*-type InP at 300 K. Experimental points (Ref. 82) are compared to Brooks-Herring theory with conventional screening (dashed curve) and to the phase-shift formalism with multi-ion screening (solid curve).

V. CONCLUSIONS

In the preceding sections, we have demonstrated that conventional derivations of the scattering potential for ionized donors in an uncompensated semiconductor overestimate the ability of free electrons to screen all impurities at the same time. From a lowest-order Kohn-Sham analysis of the single-ion problem, we have shown that low-energy electrons screen much more effectively than do high-energy electrons. Linear extrapolation to the multi-ion regime then leads to the unreasonable result that low-energy electrons contribute more charge than they possess to the total screening of all donors in the system. To overcome this difficulty, we have developed a simple, self-consistent screening formalism based on the requirement that no electron state should contribute more than $-e$ to the net screening charge.

The "multi-ion screening length" derived from this formalism has been used to obtain improved cross sections for the scattering of electrons by ionized donors. In order to test the effects of the revised scattering potentials on electron transport, we have recalculated electron mobilities for uncompensated *n*-type germanium, silicon, GaAs, and InP as a function of doping level and temperature. In several important regimes, such as low-temperature silicon, room-temperature silicon at $N_D \approx 10^{20}$ cm^{-3}, and low-temperature germanium at donor densities in the range $N_D \leq 10 n_c$, the multi-ion screening correction to the mobility is quite large. Theoretical mobilities are reduced by factors of 2 to 4, and the agreement with experiment is considerably improved. In other cases such as room-temperature germanium and GaAs and InP at 77 K, the correction is somewhat more modest but still markedly improves the agreement with experiment. On the other hand, in examples such as GaAs and InP at 300 K, where agreement between the conventional theory and experiment was already fairly good, the multi-ion correction to the mobility is much smaller. In only one case considered, low-temperature germanium at $N_D \geq 2\times10^{18}$ cm^{-3}, does the more general theory overcorrect the mobility, and there the conventional and multi-ion screening calculations are in roughly equal disagreement with experiment ($\approx 30\%$). We have encountered no example in which the multi-ion screening correction appreciably worsens the agreement between theoretical and experimental electron mobilities.

In a future work we will treat the effects of multi-ion screening on electron transport properties in a compensated semiconductor. With significant compensation the increase of the screening length will be larger since $n \ll N_I$ and it is even more difficult for a given number of electrons to screen all donors and acceptors at the same time.[16] However, it should be remembered that the electron transport is only sensitive to changes in the screening length when the parameter b [see Eq. (4.3)] is small. At small-electron densities and hence long screening lengths and large b, the direct effect of multi-ion screening on the single-site scattering cross sections is not necessarily large in compensated samples. However, we have shown previously[15] that the single-site theory is inaccurate whenever the potential fluctuations due to random inhomogeneities in the impurity density are large compared to typical electron energies. The multi-ion screening correction may therefore be quite significant in that it leads to much larger fluctuations than are estimated from the conventional screening calculation.

APPENDIX: EVALUATION OF $\rho_3(r)$ IN THE WEAK-POTENTIAL LIMIT

It is useful to rewrite the radial wave function in the form[91]

$$\frac{R_l(kr)}{kr}=\frac{\alpha_l(kr)}{\alpha_l(kr\to\infty)}[j_l(kr)\cos\hat{\delta}_l(r)-n_l(kr)\sin\hat{\delta}_l(r)] \tag{A1}$$

where n_l is the lth-order spherical Bessel function of the second kind. The "amplitude function" $\alpha_l(kr)$ is defined

$$\alpha_l(kr)=\exp\left\{-\frac{2m_e}{\hbar^2 k}\int_0^r dr'\phi_{\rm eff}(r')r'^2[j_l(kr')\cos\hat{\delta}_l(r')-n_l(kr')\sin\hat{\delta}_l(r')] \times[j_l(kr')\sin\hat{\delta}_l(r')+n_l(kr')\cos\hat{\delta}_l(r')]\right\} \tag{A2}$$

while the "phase function" $\hat{\delta}_l(r)$ satisfies the first-order differential equation

$$\frac{\partial\hat{\delta}_l(r)}{\partial r}=-\frac{2m_e k r^2\phi_{\rm eff}(r)}{\hbar^2}[j_l(kr)\cos\hat{\delta}_l(r)-n_l(kr)\sin\hat{\delta}_l(r)]^2 \tag{A3}$$

and becomes the usual phase shift at large r: $\hat{\delta}_l(r\to a)=\delta_l$. In Eq. (A1), we have normalized to $\alpha_l(\infty)$ so that the boundary condition Eq. (2.6) is satisfied at large r. The effective potential is $\phi_{\rm eff}(r)=\phi(r)+\phi_{\rm xc}$.

In the "weak-potential" limit, the phase shifts are small and Eq. (A3) yields the Born-approximation phase function [compare with Eq. (2.27) of Ref. 20]

$$\hat{\delta}_l(r)\to-\frac{2m_e k}{\hbar^2}\int_0^r\phi_{\rm eff}(r')j_l^2(kr')r'^2dr' \ . \tag{A4}$$

Similarly, the normalized amplitude function becomes

$$\frac{\alpha(kr)}{\alpha(\infty)}\to 1+\frac{2m_e k}{\hbar^2}\int_r^\infty\phi_{\rm eff}(r')r'^2 j_l(kr')n_l(kr')dr' \ . \tag{A5}$$

Substitution of these forms into Eq. (A1) leads eventually to

$$\sum_{l=0}^{\infty}(2l+1)\left[\frac{R_l^2(kr)}{(kr)^2}-j_l^2(kr)\right]\to-\frac{\phi_{\rm eff}(r)}{2\varepsilon} \ , \tag{A6}$$

where one integration has been performed by parts and we have used the result

$$\sum_{l=0}^{\infty}(2l+1)(kr)^3 j_l(kr)\{j_{l-1}(kr)[j_{l+1}(kr)n_l(kr)-j_l(kr)n_{l+1}(kr)]-j_{l+1}(kr)[j_l(kr)n_{l-1}(kr)-j_{l-1}(kr)n_l(kr)]\}$$

$$-\sum_{l=0}^{\infty}\frac{(2l+1)k^3}{\phi_{\text{eff}}(r)}\left[j_l^2(kr)\int_r^{\infty}\frac{\partial\phi_{\text{eff}}(r')}{\partial r'}r'^{\,3}[2j_l(kr')n_l(kr')-j_{l-1}(kr')n_{l+1}(kr')-j_{l+1}(kr')n_{l-1}(kr')]dr'\right.$$

$$\left.+2j_l(kr)n_l(kr)\int_0^{r}\frac{\partial\phi_{\text{eff}}(r')}{\partial r'}r'^{\,3}[j_l^2(kr')-j_{l-1}(kr')j_{l+1}(kr')]dr'\right]\approx 1\ . \qquad \text{(A7)}$$

Of the two sums over l, it is easily shown using well-known relations[92] that the first is identically unity. For $kr \gg 1$ and $[\partial\phi_{\text{eff}}(r)/\partial r]/k\phi_{\text{eff}}(r) \ll 1$ (that is, the effective potential does not vary significantly over an electron wavelength), the second sum is small and oscillating for any potential $\phi_{\text{eff}}(r)$.

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[10] Although ϕ_{xc} can be straightforwardly included using the Kohn-Sham approximation (see Ref. 5), we ignore it in the present treatment in order to allow direct comparison with previous LTF calculations. In lowest order, exchange correlation contributes a term which has the same functional form as the screened Coulomb potential. For an attractive interaction ϕ_{xc} adds to the effective strength of the potential, making the multi-ion phenomena discussed below even more important.

[11] For example, see J. S. Blakemore, *Semiconductor Statistics* (Pergamon, New York, 1962), Appendix B.

[12] While $\bar{\rho}_i(r)$ represents the average excess charge density per state, not all electrons with energy ε contribute equally to the screening of a given ion. This is because only electron states with a small quantum number l interact strongly with the impurity [see Eq. (2.11)]. However, in the next section the single-ion screening charge $\bar{\rho}_i(r)$ is summed over all the ions in the system, which leads to an averaging over l.

[13] Errors introduced into Eq. (2.16) by the retention of only linear terms in the weak-potential calculation of the Appendix will be of second order, since they effect the functional form of $\bar{\rho}_i(\mathbf{r})$ but not the basic relation that low-energy electrons contribute much more to the screening than high-energy electrons.

[14] The "left-over" charge may be thought of as providing a uniform background which preserves the overall charge neutrality of the system.

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