Ionized-impurity scattering in the weak-screening limit

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The ionized-impurity-scattering problem in free-carrier transport is considered for the regime where half the average distance between impurities, D, is much less than the screening length λ_s. Using a potential-cutoff approach, it is shown that the scattering by short-range potential variations due to the discrete positions of the ions becomes negligible in the limit $d \equiv (\lambda_s/D)^3 \gtrsim b^{3/2}/(8g)^{3/4}$, where $b = 4k^2\lambda_s^2$, k is the electron wave vector, and $g(b) = \ln(b+1) - b/(b+1)$. In this region the dominant mechanism is scattering by long-range potential fluctuations due to random inhomogeneities in the impurity concentration. A random-potential-scattering theory is used to show that, for fluctuations γ small compared with the electron energy E, the momentum relaxation time reverts to the Brooks-Herring form, even though the single-site scattering picture is formally inappropriate. It is shown that the criterion $\gamma \gtrsim E$ is nearly equivalent to the single-site validity criterion $\langle \tau_D/\tau_R \rangle \lesssim 1$ derived earlier for the small-d regime, where τ_D is the duration of the collisions, τ_R is the momentum relaxation time, and the brackets denote a weighted average over partial waves. Furthermore, at large d the linearized Thomas-Fermi approximation is valid only as long as $\gamma \lesssim E$. Whenever $\gamma \gtrsim E$, significant discrepancies between single-site theoretical mobilities and experimental values are observed for a number of common semiconductors. It is suggested that spatial inhomogeneities in the electron density due to the fluctuating potential may be partially responsible for these discrepancies.

I. INTRODUCTION

At low temperatures, ionized impurities are the dominant mechanism limiting free-carrier mobilities in most semiconductors. Calculations of ionized impurity scattering have usually been based on the assumption that the ions scatter independently of one another. This has been due in part to the absence of reliable multi-ion corrections to the electron momentum relaxation time.[1] Furthermore, until recently considerable confusion has persisted in the literature about the conditions under which the assumption of independent scattering events breaks down. Employing a criterion suggested by Rode and Knight,[2] the authors showed in an earlier work[3] (referred to below as I) that the single-site scattering model is valid only when the criterion

$$\langle \tau_D/\tau_R \rangle \lesssim 1 \tag{1.1}$$

is satisfied. Here τ_D is the duration of the collisions, τ_R is the momentum relaxation time, and the brackets denote a suitable weighted average over the various scattering events. When the partial-wave phase-shift method is used to calculate electron mobilities in Si,[4] GaAs,[5] ZnSe,[6] CdTe,[7] and InSb,[8] one finds a direct correlation between the magnitude of $\langle \tau_D/\tau_R \rangle$ and the extent to which the calculated mobilities agree with experiment.

A number of previous investigators[9] have pointed out that the assumption of independent scattering by the various ions should also fail whenever there is significant overlap of neighboring potentials. Using analytic results for scattering by screened charge pairs as a guide, the authors derived in a recent study[10] (referred to below as II) an explicit criterion for the neglect of coherent interference effects:

$$d \equiv (\lambda_s/D)^3 \lesssim 8/(1 + 64\, b^{-3/2}), \tag{1.2}$$

where $D = (4\pi N_I/3)^{-1/3}$ is half the average distance between impurities, N_I is the impurity density, λ_s is the screening length, $b \equiv 4k^2\lambda_s^2$, and k is the electron wave vector. The physical interpretation of Eq. (1.2) is easily seen if the expression is rewritten in the form

$$\left[\frac{\lambda_s}{2D}\right]^3 + \left[\frac{\lambda_e}{2\pi D}\right]^3 \lesssim 1, \tag{1.3}$$

where $\lambda_e = 2\pi/k$ is the electron de Broglie wavelength. That is, the assumption of independent scattering by neighboring ions is strictly valid only as long as the distance between ions is large compared to both the screening length λ_s and the electron wavelength λ_e. However, it is also shown in II that as long as criterion (1.1) is satisfied, theoretical single-site mobilities for relatively compensated GaAs and InSb agree well with experimental values even when criterion (1.2) is strongly violated. In the present study we examine in detail the region where criterion (1.1) is satisfied but criterion (1.2) is not. In particular, we seek to provide insight into the apparent success of the single-site theory in regions where it should clearly be invalid.

In Sec. II, the phenomenology of electron scattering in the regime $d \gg 1$ is discussed. It will be seen that an approach fundamentally different from the single-site model is required for treating the scattering in this region. In Sec. III, a random potential formalism is employed to calculate electron relaxation times at large d, and a connection between criterion (1.1) and conduction-band distortion is discussed. Finally, we consider the regime where criterion (1.1) is violated, and suggest a phenomenological explanation for the tendency of single-

site theoretical mobilities to be significantly higher than experimental values when $\langle \tau_D/\tau_R \rangle \gtrsim 1$. For simplicity, it will be assumed that the unpertured conduction band is isotropic and parabolic.

II. PHENOMENOLOGY OF SCATTERING WHEN $d \gg 1$ and $\langle \tau_D/\tau_R \rangle \lesssim 1$

It was shown in II that the single-site model ceases to be formally valid at large d [see criterion (1.2)] due to multi-ion interference effects. Here we consider two quite different approaches which have been suggested in the literature for calculating electron momentum relaxation times when d is large. The first, which was originally proposed by Conwell and Weisskopf,[11] consists of "cutting off" the potentials at a range on the order of the average ion separation, then calculating individual scattering rates due to each cut-off potential. In the second approach, which has been discussed by Yussouff and Zittartz,[12] an electron is viewed as moving through a continuously varying effective potential arising from random fluctuations in the impurity concentration. The relaxation time for "continuous" scattering by the random potential is then determined. We now briefly outline both of these approaches and discuss the connection between them.

In the linearized Thomas-Fermi approximation[13] (the validity of which is discussed in the Appendix), the net screened potential due to any number of charged ions is simply a superposition of the screened Coulomb potentials corresponding to each:

$$V(\vec{r}) = \sum_i \frac{Z_i e^2 e^{-|\vec{r}-\vec{r}_i|/\lambda_s}}{\kappa_0 |\vec{r}-\vec{r}_i|}, \tag{2.1}$$

where Z_i is the charge of the ith ion, $\vec{r}_i$ is its position, κ_0 is the static dielectric constant, and the screening length λ_s is given by[13]

$$\lambda_s^{-2} = \frac{4\pi n e^2}{\kappa_0 k_B T} \frac{\mathcal{F}_{-1/2}(\eta)}{\mathcal{F}_{1/2}(\eta)}. \tag{2.2}$$

Here n is the electron density, $\eta \equiv E_F/k_B T$ is the reduced Fermi level, and $\mathcal{F}_k$ is a Fermi integral of order k. When $d \gg 1$, it is useful to separate the sum over ions i in Eq. (2.1) into three components: (1) ions at distances $|\vec{r}-\vec{r}_i| \gg \lambda_s$, which are strongly screened and may be ignored; (2) ions at distances $D \ll |\vec{r}-\vec{r}_i| \lesssim \lambda_s$, which represent most of those contributing to $V(\vec{r})$ when d is large (on a distance scale of order D, their contribution to the potential is smooth and slowly varying in $\vec{r}$); (3) nearby ions at distances $|\vec{r}-\vec{r}_i| \lesssim D$, which lead to rapid spatial variations of the potential due to the singularities at ion sites ($\vec{r} \to \vec{r}_i$).

It may seem that since a flat potential offset does not contribute to scattering, one can ignore the slowly varying potential fluctuations from distant ions in range (2) (this assumption will be reexamined below). Several authors[11,14,15] have obtained approximate transport results by cutting off the potential due to each ion at a distance on the order of D and then calculating individual scattering rates. Although Conwell and Weisskopf[11] and Ridley[15] treated the problem classically using the Rutherford scattering formalism, it seems more appropriate to perform a quantum-mechanical calculation such as that of Sclar.[14] He obtained the first four phase shifts for scattering by a square well (attractive) or square barrier (repulsive) potential. For the region $d \gg 1$ he set the width of the well or barrier to be $a = b'D$, where b' is a constant on the order of unity. The well depth or barrier height is then taken to be $\pm e^2/\kappa_0 a$.

Here we give a slightly different result which is obtained in the Born approximation assuming a cutoff bare Coulomb potential,[16] and which has a somewhat simpler form than that of Sclar. It can be shown that if the potential is cut off at D (i.e., $b' = 1$), one obtains for the momentum-transfer scattering cross section

$$\sigma_{co}(k) = \frac{\pi}{y^2 k^2} \{2[\gamma + \ln(2kD) - \mathrm{Ci}(2kD)] - \tfrac{1}{2}[\gamma + \ln(4kD) - \mathrm{Ci}(4kD)]\} \tag{2.3}$$

which is the same for either attractive or repulsive potentials. Here $\gamma = 0.5772\ldots$ is Euler's constant, $y \equiv \frac{1}{2} k a_0$, $a_0 = \hbar^2 \kappa_0/m_e e^2$ is the effective Bohr radius, m_e is the electron effective mass, and Ci is the cosine integral.[17] In the limit $kD \ll 1$, this result can be written

$$\frac{\sigma_{co}(k)}{\sigma_{BH}(k)} = \frac{2(kD)^4}{g(b)} = \frac{b^2}{8d^{4/3} g(b)}, \tag{2.4}$$

where σ_{BH} is the Brooks-Herring cross section for scattering by a screened Coulomb potential[18]

$$\sigma_{BH}(k) = \frac{\pi}{2k^2 y^2} g(b) \tag{2.5}$$

and $g(b) \equiv \ln(b+1) - b/(b+1)$. In this limit Sclar's result is smaller than the present σ_{co} by a factor of $\frac{4}{9}$ due to his use of a square well or barrier rather than a cutoff bare Coulomb potential. In the opposite limit $kD \gg 1$,

$$\frac{\sigma_{co}}{\sigma_{BH}} = \frac{1}{g}[\gamma + \ln(b^{3/2}/2d)]. \tag{2.6}$$

It can be shown that as long as $d > 1$, one never obtains $\sigma_{co}/\sigma_{BH} > 1$.

Relation (2.4) indicates that the scattering by short-range interactions is reduced below the usual Brooks-Herring value whenever

$$d \gtrsim \frac{b^{3/2}}{[8g(b)]^{3/4}} \tag{2.7}$$

(which for $b \gtrsim 1$ is approximately equivalent to $kD \lesssim 1$). Relation (2.7) implies that the distance between impurities is shorter than both the screening length and the electron wavelength. If one considers only the short-range potential variations, the calculated electron mobility actually increases with increasing impurity density when d is sufficiently large.[19]

The second approach we consider for obtaining relaxation times in the region $d \gg 1$ is based on the scattering

by long-range potential fluctuations which result from random inhomogeneities in the impurity concentration. Although the results of a formal theory for this mechanism[12] will be discussed in the next section, we first estimate the magnitude of the effect from phenomenological considerations.

For simplicity, we consider an uncompensated impurity population consisting only of singly charged donors of density N_D. In the limit $d \gg 1$, a test electron "interacts" with an average of $N \approx 4\pi N_D \lambda_s^3/3 = d$ ions at a time (screening greatly reduces the effect of any ions farther than λ_s away from the electron). Since the donors are very closely packed and since each contributes a negative potential energy, one result of these interactions is a lowering of the effective bottom of the conduction band. It can easily be shown that to within a multiplicative constant the average potential energy is given by $V_0 = -Ne^2/\kappa_0\lambda_s$, where $V = 0$ is taken to be the unperturbed bottom of the band in the absence of impurities. It was pointed out above that were this background offset a constant everywhere, no scattering by the long-range interactions would result. However, the actual V_0 varies with position due to random variations in the donor density. For Gaussian statistics the fluctuations in N are of magnitude $N^{1/2}$, which implies that the offset potential should display fluctuations of order[20,21] $N^{1/2}e^2/\kappa_0\lambda_s$.

To a first approximation the scattering due to a given fluctuation may be estimated by calculating the cross section for a square well (or barrier) of radius $a = \lambda_s$ and depth (or height) $V = N^{1/2} e^2/\kappa_0\lambda_s$. In the Born approximation one obtains[22]

$$\sigma_F = \frac{16\,\pi^2 N_D \lambda_s^3}{3(ky)^2}\, h(b), \tag{2.8}$$

where

$$h(b) = \frac{\sin(2b^{1/2})}{2b^{1/2}} - \frac{1}{2} - \frac{1-\cos(2b^{1/2})}{4b} + \tfrac{1}{2}\left[\gamma + \ln(2b^{1/2}) - \mathrm{Ci}(2b^{1/2})\right] \tag{2.9}$$

and Ci is again the cosine integral. The inverse momentum relaxation time for scattering from the fluctuations may then be obtained from the expression $\tau_F^{-1} \approx N_F\, v\, \sigma_F$, where v is the electron velocity and the "density" of fluctuations is the inverse of the volume of each: $N_F \approx 3/4\pi\lambda_s^3$. Comparing with the Brooks-Herring result for single-site scattering from a screened Coulomb potential one obtains

$$\frac{\tau_F^{-1}}{\tau_{BH}^{-1}} \approx \frac{N_F\, v\sigma_F}{N_D\, v\sigma_{BH}} = \frac{h(b)}{g(b)}. \tag{2.10}$$

Evaluation of h and g shows that $\tau_F^{-1}/\tau_{BH}^{-1}$ varies only between $\frac{4}{9}$ for $b \ll 1$ and 2 for $b \gg 1$. That is, to within roughly a factor of 2, we predict that the relaxation time due to scattering by long-range fluctuations is equal to the usual single-site value one obtains if each of the ions is assumed to scatter independently. This result is easily generalized to the case of arbitrary compensation. It should be remembered that since the simple phenomenological calculation has treated the fluctuations as a perturbation of the bottom of the conduction band, the model will break down if the fluctuations become too large.

For cases where $\langle \tau_D/\tau_R \rangle \lesssim 1$ we have discussed two distinct approaches for treating ionized impurity scattering in the region $d \gg 1$, where the single-site model is formally invalid due to interference effects. The results obtained are not at all similar because the two approaches treat different aspects of the problem. In the first, only short-range potential variations ($r \lesssim D$) due to the discrete positions of the ions are considered. If the potential due to each impurity is cut off at $r = D$, one finds that the "individual ion" contribution to the scattering is quite small in the large-d limit where criterion (2.7) is satisfied. The second approach considers only the long-range potential fluctuations ($D \ll r \lesssim \lambda_s$) due to random inhomogeneities in the impurity concentration. By treating each fluctuation as a square well we found that to a first approximation, the momentum relaxation time is the same as the Brooks-Herring value for scattering by individual screened Coulomb centers. One should therefore not expect to observe experimentally the large mobility increases predicted by Eq. (2.4) for the case where criterion (2.7) holds and only short-range interactions are considered. In the next section we discuss a detailed theory[12] for calculating the scattering by random long-range fluctuations. Since short-range potential variations will be ignored, the calculation is strictly valid only when criterion (2.7) is satisfied.

III. RANDOM-POTENTIAL-SCATTERING THEORY

Yussouff and Zittartz (YZ) have treated the "continuous" scattering of an electron by a smoothly varying random potential.[12] They employed a memory-function technique in lowest order, which is valid as long as the potential fluctations are smaller than the electron energy. The energy-dependent momentum relaxation time $\tau_{YZ}(E)$ was found to have the form

$$\tau_{YZ}^{-1}(E) = \frac{1}{2^{9/2}\,\pi\, m_e^{1/2} E^{3/2}} \times \int_0^\infty q^3\, D(q)\, \mathrm{erfc}\left[\frac{E_q/4 - E}{\gamma}\right] dq, \tag{3.1}$$

where erfc is the complimentary error function,[23] $E_q \equiv \hbar^2 q^2/2m_e$, γ is $2^{1/2}$ times the rms potential energy,[24] and $D(q)$ is the Fourier transform of the potential correlation function

$$W(\vec{r} - \vec{r}') = \langle V(\vec{r})\, V(\vec{r}') \rangle = \sum_i \frac{1}{\Omega} \int d^3r_i\, V_i(\vec{r}_i - \vec{r})\, V_i(\vec{r}_i - \vec{r}'). \tag{3.2}$$

Here Ω is the volume, $V_i(\vec{r})$ is the potential due to the ith impurity, and we have assumed that the impurity positions are uncorrelated. For a given potential distribution, γ may be found from the relation $\gamma^2 = 2W(0)$.

Yanchev *et al.*[25] have applied the YZ formulation to the case of a screened Coulomb form for the impurity po-

tentials, i.e., $V_i(\vec{r}) = -Z_i e^2 e^{-r/\lambda_s}/\kappa_0 r$. For singly charged impurities ($|Z_i| = 1$) they obtain

$$W(\vec{r}) = 2\pi N_I e^4 \lambda_s e^{-r/\lambda_s}/\kappa_0^2 \tag{3.3}$$

which implies

$$D(q) = \frac{16\,\pi^2 N_I e^4}{\kappa_0^2 (q^2 + \lambda_s^{-2})^2} \tag{3.4}$$

and

$$\gamma^2 = \frac{4\pi N_I e^4 \lambda_s}{\kappa_0^2}. \tag{3.5}$$

It is useful to compare τ_{YZ}^{-1} with the Brooks-Herring result τ_{BH}^{-1} for scattering by individual screened Coulomb potentials in the Born approximation:

$$\frac{\tau_{YZ}^{-1}(E)}{\tau_{BH}^{-1}(E)} = \frac{1}{2g}\int_0^\infty \frac{u\,du}{(u+\delta)^2}\,\mathrm{erfc}\left[\frac{u}{4} - \beta^{-1/2}\right], \tag{3.6}$$

where we define the dimensionless parameters

$$\delta = \frac{\hbar^2 \lambda_s^{-2}}{2m_e\gamma} \rightarrow \frac{2y}{(3bd)^{1/2}} \tag{3.7}$$

and

$$\beta = \frac{\gamma^2}{E^2} \rightarrow \frac{12\,d}{by^2} \tag{3.8}$$

[g is defined following Eq. (2.5) and y is defined following Eq. (2.3)]. Figure 1 shows a plot of $\tau_{YZ}^{-1}/\tau_{BH}^{-1}$ vs β for $\delta = 0.001$ and 0.1. The ratio is very nearly unity for small β, i.e., whenever the average fluctuation is small compared to the electron energy. As β increases, $\tau_{YZ}^{-1}/\tau_{BH}^{-1}$ falls below unity, reaching values at $\beta = 3$ of 0.80 and 0.83 when $\delta = 0.001$ and 0.1, respectively. Although the figure shows the ratio eventually increasing for $\delta = 0.1$ at sufficiently large β, the lowest-order calculation of Yussouff and Zittartz is invalid in the large-β regime.

We find that as long as the criterion

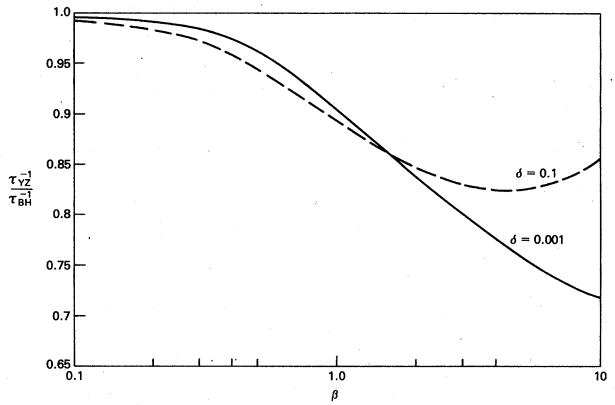

FIG. 1. Ratio of the Yussouff and Zittartz inverse relaxation time to the Brooks-Herring result. Here $\beta \equiv \gamma^2/E^2$ and $\delta \equiv \hbar^2\lambda_s^{-2}/2m_e\gamma$, where γ is the typical magnitude of the potential fluctuations.

$$\tfrac{1}{3}\beta = \frac{4d}{by^2} \lesssim 1 \tag{3.9}$$

is satisfied, the two inverse relaxation times are nearly equal. This is despite the fact that one result (τ_{BH}^{-1}) has been obtained assuming scattering by individual ions while the other (τ_{YZ}^{-1}) is based on collective scattering by long-range potential fluctuations due to random inhomogeneities in the impurity concentration. We have verified the conclusion reached phenomenologically in the previous section that although the potential fluctuation approach is more appropriate physically when $d \gg 1$, as long as the fluctuations are small the resulting scattering is similar for the two ways of treating the problem. On the other hand, when $\frac{1}{3}\beta \gtrsim 1$ [criterion (3.9) is violated], the Brooks-Herring result ceases to be "accurate."

It is useful to compare this relation with criterion (1.1) for the validity of the single-site scattering approximation in the regime where interference effects are negligible [i.e., small d, as specified by criterion (1.2)]. It can be shown using Eq. (3.4) and Fig. 2 of I that whenever b and y are not too small $\langle \tau_D/\tau_R \rangle \approx 4d/by^2$, i.e., criteria (1.1) and (3.9) are nearly identical. (For cases of experimental interest such as those discussed in I, this relation usually holds to better than 30%.) This apparent equivalence of criteria resulting from different physical considerations can be attributed to the fact that both are related to the breakdown of the free-electron quasiparticle picture.[26] Criterion (1.1) is violated when the momentum relaxation time is short compared to the average duration of the collisions, i.e., the states are damped on a time scale short compared to other relevant times in the transport problem.[27] Similarly, criterion (3.9) is violated when the magnitude of the potential fluctuations is large compared to the electron energy, i.e., the distortion of the conduction band is too large for the states at the bottom of the band to be considered perturbed free-electron states. In both cases, the electron wave vector k ceases to be a "good" quantum number.[26] Before proceeding we further note that criterion (A9) in the Appendix for the validity of the linear net ion potential Eq. (2.1) is also nearly identical to criterion (3.9) whenever d is large. The "linearization" of the Thomas-Fermi screening charge density breaks down whenever the electron screening charge induced by the ion potentials becomes too large to be treated by a linear expansion. This occurs when the potential energy fluctuations are comparable to the kinetic energy.

It was shown in I that when criterion (1.1) is violated for semiconductors such as silicon, GaAs, and ZnSe at low temperatures, theoretical mobilities based on the partial-wave phase-shift method usually exceed the experimental values, often by a factor of 2 or more. However, Fig. 1 illustrates that mobilities calculated from the lowest-order random potential theory[12] will be even higher than those obtained using the single-site approach. That is, the correction is in the wrong direction to explain the discrepancy between the single-site theory and experiment. It appears that the YZ theory ignores additional phenomena which become important in the same region and tend to decrease the observed mobility. Shklovskii and Éfros have pointed out that for a distorted conduction band

with spatial fluctuations, the electrons preferentially populate those locations with the lowest potential energy.[28] This causes a general lowering of the Fermi level and a decrease in the mobility due to the smaller electron energies. Furthermore, the resulting inhomogeneities in the electron density lead to an electrical conductivity $\sigma(\vec{r})$ which varies with position.[28] Dykhne has shown that the effective conductivity σ_s for an inhomogeneous medium of total extent large compared to the dimensions of the fluctuations falls in the range[29] $\langle \sigma^{-1} \rangle^{-1} \leq \sigma_s \leq \langle \sigma \rangle$, where the brackets denote a spatial average. That is, σ_s is always less than the "average" conductivity $\langle \sigma \rangle$. In the limit of extremely large fluctuations one can in principle obtain σ_s orders of magnitude below $\langle \sigma \rangle$, since virtually all of the electrons will be frozen into isolated "droplets" at positions where the potential energy is lowest.[28]

Although some aspects of the transport problem with potential fluctuations have been discussed by Shklovskii and Éfros[28] and others,[30] their percolation theory analysis is unsuitable for treating the regime of present interest, since it is directed primarily toward the study of impurity conduction and the transition between metallic and activated conductivities. However, preliminary numerical evaluations[31] of more accurate expressions[32] for σ_s show that simply by accounting for the inhomogeneity of the conductivity and the shift in the Fermi energy, one obtains corrections to the effective electron mobility which are of roughly the appropriate magnitude to improve the agreement between theory and experiment at low temperatures when $4d/by^2 \gtrsim 1$. This type of calculation may be considered a first step toward unifying the $\gamma \ll E$ regime where the free-electron picture is appropriate and the $\gamma \gg E$ regime where conduction-band distortion effects dominate and most of the relevant electron states are localized. Ultimately, a proper treatment[33] must account for the fact that electrons in the two regions are characterized by wave functions and densities of states, as well as screening and scattering processes that are qualitatively different.[26]

IV. DISCUSSION

It was mentioned above that the single-site model for electron scattering by ionized impurities breaks down whenever $\langle \tau_D/\tau_R \rangle \approx 4d/by^2 \gtrsim 1$, i.e., the lifetime that an electron spends in a given state is short compared to the duration of the collisions. In that region, significant discrepancies are generally obtained between results of the single-site scattering theory and experiment. We also examined the phenomenology of charged-center scattering in the region $d \gg 1$, i.e., many impurities are contained within a sphere of radius λ_s and substantial overlap of neighboring potentials occurs. Figure 2 illustrates the regions of validity for various transport models via a two-dimensional "map" plotting the coordinates $\ln(4d/by^2)$ vs $\ln d$. In this space, the single-site model is invalid in the shaded upper half plane for which $4d/by^2 \gtrsim 1$. Note that the cross-hatched[34] area $4d/by^2 \lesssim 4/81d$ of the figure may be neglected in the present discussion, since it is never encountered when ionized impurity scattering dominates the electron transport in thermal equilibrium.

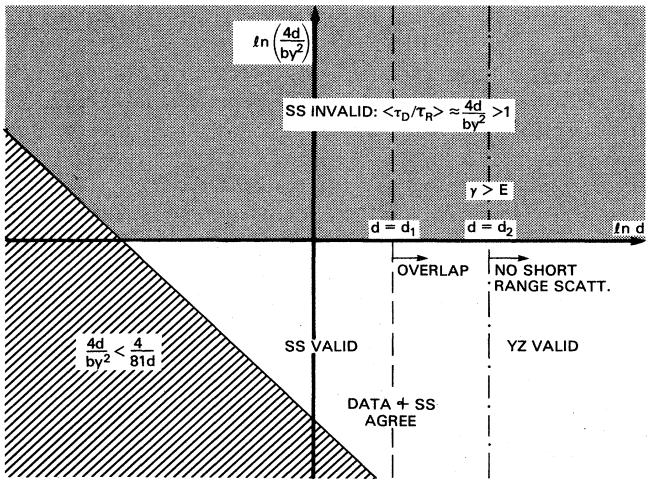

FIG. 2. "Map" of validity regions and for various transport models, assuming constant $b \gg 1$. SS is single-site theory and d_1 and d_2 are defined in the text. The cross-hatched area may be neglected because $n > N_I$ there.

According to criterion (1.2), even in the region below the abscissa the single-site theory is not formally valid when $d \gtrsim d_1 \equiv 8/(1 + 64b^{-3/2})$, i.e., to the right of the vertical dashed line in the figure. This is because coherent interference effects dominate the scattering if neighboring potentials significantly overlap one another.[10] We thus find that the triangle at the center of the figure is the only region for which the single-site model is formally valid in cases of physical interest. It can be shown that within this region, electron mobilities calculated by the partial-wave phase-shift method assuming a screened Coulomb potential generally agree well with experiment[3] as long as the linearized Thomas-Fermi approximation is valid (see the Appendix). It is difficult to treat the region $d > d_1$, since both short-range interactions due to the discrete positions of individual ions and "collective" long-range potential fluctuations are important. However, it was seen above in Sec. II that the scattering by short-range interactions becomes negligible whenever $d \gtrsim d_2 \equiv b^{3/2}/[8g(b)]^{3/4}$, that is, to the right of the dash-dot line in the figure. In this region one may employ the theory of Yussouff and Zittartz[12] to calculate the relaxation time for scattering by long-range potential fluctuations due to random inhomogeneities in the impurity density. As discussed in Sec. III, as long as $4d/by^2 \lesssim 1$ this theory yields the same electron relaxation time that one obtains from the single-site Brooks-Herring theory even though the two theories are based on quite different phenomenological considerations. While the YZ approach yields theoretical results below the abscissa for $d > d_2$, this region is not easily attained in real materials.[35] Nonetheless, the YZ calculation is quite useful in that it allows one to interpolate to the intermediate region $d_1 < d < d_2$, which is of great interest but is difficult to treat theoretically in a rigorous way. Because the single-site theory yields reasonable scattering rates for both small and large d as long as one remains below the abscis-

sa, it seems probable that the same theory would also work well for intermediate d.[36] This conjecture appears to be verified experimentally by the comparison of single-site theoretical mobilities with experimental values for compensated GaAs and InSb. It was shown in II that when $4d/by^2 \lesssim 1$ the agreement is quite good in cases corresponding to intermediate d for which as many as 35–100 ions are contained within a sphere of radius λ_s, i.e., the overlap of the ion potentials is severe.

Let us now consider the shaded region above the abscissa. When $4d/by^2 \gtrsim 1$, both single-site calculations[4–8] and the random-potential-scattering theory of Yussouff and Zittartz[12] are invalid and yield electron mobilities which tend to significantly exceed the experimental values. The first-order YZ calculation breaks down because the magnitude of the fluctuations becomes large compared to the electron energy and also because the potential employed in the theory is invalid above the abscissa (see the Appendix). In fact, no present transport theory is reliable above the abscissa for any d. Although a rigorous calculation would be extremely difficult due to the complexity of the problem, some progress may be possible if one accounts for the preferential population by electrons of those spatial locations where the fluctuating potential is lowest. This leads to a lowering of the Fermi level as well as inhomogeneities in the conductivity,[28] both of which are expected to contribute to a decrease in the net conductivity. The incorporation of these considerations into a transport theory will be the subject of a future work.

APPENDIX: VALIDITY CONDITION FOR LINEARIZATION OF THE THOMAS-FERMI CHARGE DENSITY IN POISSON'S EQUATION

The Thomas-Fermi charge density induced by a potential $V(\vec{r})$ at a given spatial location $\vec{r}$ has the form

$$\rho(\vec{r}) = -e\,[n(\vec{r}) - n_0] = -e\,N_c\left[\mathcal{F}_{1/2}\left(\eta - \frac{V - V_0}{k_BT}\right) - \mathcal{F}_{1/2}(\eta)\right], \tag{A1}$$

where $n(\vec{r})$ is the local electron density, n_0 is the average electron density, N_c is the conduction-band effective density of states, and V_0 is the average potential offset

$$V_0 \equiv \frac{1}{\Omega}\int d^3r\, V(r) \rightarrow 4\pi\,(N_D - N_A)\lambda_s^2 e^2/\kappa_0. \tag{A2}$$

The linearization approximation consists of terminating the expansion[13]

$$\mathcal{F}_{1/2}\left(\eta - \frac{V - V_0}{k_BT}\right) \rightarrow \mathcal{F}_{1/2}(\eta) - \frac{V - V_0}{k_BT}\mathcal{F}_{-1/2}(\eta) + \frac{1}{2}\left(\frac{V - V_0}{k_BT}\right)^2\mathcal{F}_{-3/2}(\eta) - \cdots \tag{A3}$$

after the linear term in $V - V_0$. Use of the linearized charge density in Poisson's equation leads to the solution represented by Eq. (2.1) for the net screened potential due to all the ions.

The linearization of Eq. (A3) is valid as long as[37]

$$\frac{1}{2}\frac{(V - V_0)}{k_BT}\frac{\mathcal{F}_{-3/2}}{\mathcal{F}_{-1/2}} \lesssim 1. \tag{A4}$$

At small d (not much overlap of neighboring ion potentials), Eq. (A4) is equivalent to the requirement that the potential energy for a given ion evaluated at distances on the order of the screening length be small compared to the electron's kinetic energy:

$$\frac{e^2}{\kappa_0\lambda_s} \lesssim \frac{\hbar^2k^2}{2m_e}. \tag{A5}$$

If both sides of the inequality are squared, Eq. (A5) may be written in the form

$$\frac{4}{by^2} \lesssim 1, \tag{A6}$$

where the dimensionless parameters b and y are defined in the text. In the opposite limit of severe potential overlap ($d \gg 1$), one is primarily concerned with whether the fluctuations about V_0 are too large. Using $V_f = \gamma/2^{1/2}$ for the rms magnitude of the fluctuations [where γ is given by Eq. (3.5)], substitution into Eq. (A4) yields the condition

$$\frac{1}{2}\frac{V_f}{k_BT}\frac{\mathcal{F}_{-3/2}}{\mathcal{F}_{-1/2}} \rightarrow \left(\frac{27\,d}{8\,by^2}\right)^{1/2}\frac{\mathcal{F}_{1/2}\mathcal{F}_{-3/2}}{\mathcal{F}_{-1/2}^2} \lesssim 1, \tag{A7}$$

where we have substituted $\hbar^3k^2/2m_e \rightarrow \frac{3}{2}k_BT\mathcal{F}_{1/2}/\mathcal{F}_{-1/2}$ for the typical kinetic energy. Squaring of both sides of the inequality then leads to the condition

$$\frac{27}{32}\frac{\mathcal{F}_{1/2}\mathcal{F}_{-3/2}}{\mathcal{F}_{-1/2}^2}\left(\frac{4d}{by^2}\right) \lesssim 1. \tag{A8}$$

It can be shown that for all η, $\mathcal{F}_{1/2}\mathcal{F}_{-3/2}/\mathcal{F}_{-1/2}^2$ varies only between unity at $\eta \ll 0$ and $\frac{1}{3}$ at $\eta \gg 0$, i.e., (A8) is nearly equivalent to $4d/by^2 \lesssim 1$.

It is convenient to combine the small- and large-d results (A6) and (A7) into the form

$$\frac{4(d+1)}{by^2} \lesssim 1. \tag{A9}$$

At large d, criterion (A9) for the validity of the linearized Thomas-Fermi approximation is equivalent to (3.9) for the validity of the YZ theory (both are based on the requirement that the potential fluctuations be small compared to the electron kinetic energy). However, at small d, criterion (A9) is generally a more severe restriction than criterion (1.1) for the free-electron quasiparticle picture, i.e., $\langle \tau_D/\tau_R \rangle \approx 4d/by^2 \lesssim 1$. Regions therefore exist where the single-site picture is valid but the linearized Thomas-Fermi approximation is inadequate.

[1]It is shown in Ref. 3 below that in most regions of present interest, the multi-ion theories of E.J. Moore, Phys. Rev. **160**, 607 (1967); **160**, 618 (1967); and of Yu. D. Arbuzov and V.M. Evdokimov, Phys. Status Solidi B **92**, 579 (1979); Fiz. Tverd. Tela (Leningrad) **22**, 535 (1979) [Sov. Phys. Solid State **22**, 316 (1979)] are invalid.

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[19]At $kD \ll 1$, σ_{co} from Eq. (2.3) is proportional to $D^4 \sim N_I^{-4/3}$ and is independent of k. Since the mobility μ is proportional to $\tau \sim (N_I\sigma)^{-1}$, one obtains $\mu \sim N_I^{1/3}$. Sclar obtained mobilities which increased with N_I in some of his examples.

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[24]In the literature (e.g., Refs. 24 and 29 below), γ is sometimes incorrectly referred to as the rms potential energy. It is convenient to include the factor of $2^{1/2}$ in the definition of γ since it allows the potential distribution function to be written in the form $F(V) = e^{-V^2/\gamma^2}/\pi^{1/2}\gamma$. The parameter u defined in Ref. 12 is the actual rms potential $\gamma/2^{1/2}$.

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[33]Although the large body of published work on the "Mott transition" [e.g., see N.F. Mott, Adv. Phys. **21**, 785 (1972)] deals with some of the same effects, it is not directly applicable since that phenomenon is generally taken to occur within an impurity band split off from the conduction band.

[34]The condition follows whenever we constrain the electron density n to be smaller than the ion density N_I (i.e., the intrinsic carrier density is negligible and there is no optical or electrical injection). We have employed the relations

$$d \equiv (\lambda_s/D)^3 \approx \tfrac{1}{9}\, b^{1/2} y \left[\frac{N_I}{n}\right]$$

and

$$\frac{\hbar^2 k^2}{2m_e} \approx \frac{3k_B T}{2} \frac{\mathcal{F}_{1/2}(\eta)}{\mathcal{F}_{-1/2}(\eta)}$$

which hold for arbitrary electron degeneracy as long as the electron temperature is equal to the lattice temperature.

[35]For InSb, these criteria require highly compensated material with $N_I > 10^{18}$ cm^{-3}. In silicon, over 10^{23} ions cm^{-3} would be required, which is of course unreasonable.

[36]More physically, the fact that the transition rate per ion is the same at small d (where the scattering is by individual ions) as it is at large d (where the scattering is by collective long-range fluctuations) implies that the rate is also likely to be comparable at intermediate d, where one has some combination of the two types of scattering.

[37]A numerical solution of the nonlinear Poisson's equation for a single ion [see J.R. Meyer, Phys. Rev. B **20**, 1762 (1979)] shows that corrections to the linear screened form tend to be relatively modest as long as the validity condition (A6) is not too strongly violated.