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Theory of screening and electron mobility: Application to *n*-type silicon

B. A. Sanborn and P. B. Allen
Department of Physics, State University of New York at Stony Brook, Stony Brook, New York 11794-3800

G. D. Mahan
Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200
and Solid State Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6030

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The dielectric function for semidegenerate *n*-type silicon is calculated in both the random-phase approximation (RPA) and the Singwi-Tosi-Land-Sjölander (STLS) approximation in a study of linear screening theory and electron mobility. Using a spherical effective-mass model for the six conduction-band valleys, the Boltzmann equation is solved exactly for phonon plus impurity scattering and the resulting mobility is compared with experiment. Significant differences are found in doped silicon at nonzero temperatures between Boltzmann equation solutions in the RPA Born approximation and the less accurate force-force correlation function formula for the electrical resistivity due to electron-impurity scattering. Phonon scattering has only secondary importance and is treated by standard deformation-potential models. The problem of scattering by linearly screened ionized impurities is treated with exact phase-shift scattering theory. RPA phase-shift calculated electron mobilities in *n*-type silicon at 300 and 77 K agree more closely with experiment than the Born approximation or Thomas-Fermi calculations. The local field correction to RPA screening of impurity potentials is not significant in scattering cross sections when the electron-electron vertex function is included. However, assuming full ionization, the STLS dielectric function yields negative electronic compressibilities at 77 K in a concentration region centered approximately where the metal-insulator transition takes place at $T=0$, and coinciding with strong violations of the Friedel sum rule by linearly screened potentials. Strong Coulomb interactions are indicated and imply an inadequacy of linear screening theory, the Born approximation, and the Boltzmann equation for electron-impurity scattering applied to the electron-gas model for doped silicon at low temperature, despite apparently good agreement with experiment.

I. INTRODUCTION

Carrier mobility in heavily doped semiconductors is limited primarily by scattering from ionized impurities. This paper presents a study of impurity potential screening and electron mobility in uncompensated *n*-type silicon at 300 and at 77 K for the $10^{18}-10^{20}$-cm^{-3} concentration range. For comparison, the screening of ionized impurities has been calculated both from the temperature-dependent random-phase approximation (RPA) dielectric function and in the linearized Thomas-Fermi approximation (LTFA). Mobilities have been obtained by numerically solving the Boltzmann equation using as input electron-impurity scattering cross sections derived with the partial-wave phase-shift method. For comparison, the Born-approximation results have been calculated also. Deformation-potential matrix elements were used to account for intravalley and intervalley scattering of electrons by phonons. Because recent work indicates that electron-electron scattering is not significant in *n*-type silicon,[1,2] it has not been included here. The results show that the RPA-phase-shift calculation of the electron-impurity contribution yields mobilities that agree more closely with experiment than LTFA results do, even when the Friedel sum rule is used to optimize the Thomas-Fermi screening length. Also presented are results of a calculation of the temperature-dependent Singwi-Tosi-Land-Sjölander (STLS) approximation to the dielectric function for *n*-type silicon.[3,4] Inclusion of exchange and correlation effects through this generalization of RPA screening of impurity potentials does not change the mobility significantly. However, it permits a study of the compressibility which shows divergent behavior at 77 K. Negative electronic compressibilities for the interacting electron gas are found to coincide with strong violations of the Friedel sum rule by linearly screened impurity potentials. An examination of the validity of linear screening theory and the Boltzmann equation suggests that the theory is not reliable under these conditions and the good agreement with experiment may be accidental.

The model used here treats a doped semiconductor as a gas of conducting electrons with a neutralizing background provided by the ionized donors. All impurities are assumed to be ionized. Effects of the band structure of silicon are included simply by using the appropriate interband dielectric constant $\epsilon_\infty = 11.7$, conduction-band valley degeneracy $n_{\text{val}} = 6$, and the density of states and conductivity effective masses $m^* = 0.33$ and $m_c = 0.268$, respectively. Spherical energy surfaces are assumed throughout the calculations. Correlations between successive scatterings from different impurities are ignored.

An impurity is viewed as a weak external potential with Fourier components $\phi_{\text{ext}}(q)=4\pi Ze/\epsilon_\infty q^2$, where Ze is the impurity charge. Results presented in this paper are for $Z=1$, that is, for singly charged positive ions. The induced density response $\delta n(q)$ is assumed to be proportional to $\phi_{\text{ext}}(q)$. Screening is thus determined by the static longitudinal dielectric function $\epsilon(q)$ defined in linear response theory and the screened potential is $\phi(q)=\phi_{\text{ext}}(q)/\epsilon(q)$.

The Friedel sum rule places a condition on a screened impurity potential: the screening charge must exactly cancel the ionized impurity charge. For n-type semiconductors, it has the following form:[5,6]

$$Z=\frac{2n_{\text{val}}}{\pi k_B T}\sum_l (2l+1)\int_0^\infty \delta_l(E)f(E)[1-f(E)]dE \ . \tag{1}$$

Here $\delta_l(E)$ is the phase shift of the wave function for the scattering electron with angular momentum l and energy E, $f(E)$ is the Fermi-Dirac distribution function, T is the temperature, and k_B is Boltzmann's constant. Equation (1) is valid even when bound electronic states exist, as long as the impurity potentials are not overlapping. Fortunately, the sum rule is most robust in the region of strong screening, where it is most useful for the present analysis. The results presented here show that an impurity potential screened in linear-response theory violates the rule especially when it is just strong enough to form its first bound state. It is argued that strong violations of the Friedel sum rule are signals of the breakdown of linear screening theory.

Electron exchange and correlation contributions to screening yield a local-field correction (LFC) to the RPA dielectric function which is significant when electron-electron coupling is strong. These effects have been included in the present study through the temperature-dependent STLS approximation.[3,4] The LFC appears unimportant in the electron-test charge interaction when the electron-gas model is assumed, but it can introduce major changes in thermodynamic properties. Though the dielectric function $\epsilon(q)$ describes screening only in the linear approximation, it exactly describes the electron-electron interaction energy which determines the free energy of the gas. The compressibility sum rule relates the long-wavelength static dielectric function to the isothermal electronic compressibility K at electron density n,[7]

$$\lim_{q\to 0}\epsilon(q,0)=1+\frac{4\pi e^2}{\epsilon_\infty q^2}n^2K \ . \tag{2}$$

For stability of a system, K is required to be positive, but a negative electronic contribution seems to be permitted. Negative compressibilities have been predicted for the zero-temperature interacting electron gas at densities lower than a critical value by several LFC theories[8,9] and by Monte Carlo calculations.[10] Also in the classical limit, negative compressibilities have been found with LFC dielectric functions[11,12] and Monte Carlo methods.[13] An experimental measurement[14] of negatively divergent compressibilities in the two-dimensional electron gas has been reported for densities lower than a critical value, in good qualitative agreement with Monte Carlo[15] and STLS (Ref. 16) calculations. The compressibility sum rule applied to the STLS dielectric function correctly predicts that negative values of K occur in all of these cases, though it tends to underestimate the critical coupling strength somewhat. It is generally agreed that the negative K values do not signal an instability of the electron gas since the neutralizing background is able to stabilize the system.[13]

More recently, Tanaka and Ichimaru[17] found a region in the density-temperature plane corresponding to negative isothermal compressibilities. One may then ask whether this behavior occurs for nonzero temperatures and densities relevant to the study of transport in doped semiconductors. We find that K diverges when the magnitude of the electron-electron interaction energy is equal to the average kinetic energy of the interacting electrons. Application of the compressibility sum rule to the STLS dielectric function for n-type silicon shows that at low enough temperatures the interacting gas compressibility and the long-wavelength static electric polarizability diverge. At 77 K, the ratio of the noninteracting gas compressibility, K_{free}, to K is negative for a broad range of electron concentrations and is minimum near the density where the impurity potential forms its first bound state, approximately coinciding with the density where the metal-insulator transition takes place at $T=0$. Though we know of no previous calculation of divergent compressibilities in a real bulk semiconductor, it is perhaps not surprising that they should appear near the metal-insulator transition where strong coupling effects are expected to be important. Divergent donor polarizabilities were observed experimentally[18] in insulating samples of phosphorous-doped silicon as the metal-insulator transition was approached.

It is interesting that the quantities under study, such as the Friedel sum rule violation, compressibility, and Coulomb coupling strength, are not monotonic functions of density for fixed temperature. This is related to the fact that doped silicon falls between the classical and degenerate limits of the electron-gas model into the region of semidegeneracy. The degree of degeneracy of an electron gas may be characterized by the dimensionless temperature $\Theta=k_BT/E_F$. In a doped multiple-valley semiconductor such as silicon or germanium, the Fermi energy $E_F=\hbar^2/2m^*(3\pi^2n/n_{\text{val}})^{2/3}$ is smaller than it would be in a single-valley band at the same electron density. Multiple valleys push a semiconductor in the direction of nondegeneracy. Dandrea, Ashcroft, and Carlsson[19] found that $\Theta<0.1$ approximately defines the degenerate regime, while $\Theta>10-100$ defines the nondegenerate or classical regime. They found that for $0.1<\Theta<10$, the electron gas is semidegenerate and inadequately described by either zero-temperature or classical theories. In silicon at room temperature, Θ varies from 7.7 for an impurity concentration of 10^{18} cm^{-3} to 0.36 for 10^{20} cm^{-3}, putting heavily doped silicon squarely into the region of semidegeneracy. Clearly, a screening model must be valid in this region if it is to describe accurately the screening of impurities in doped semiconductors.

The screening capability of a system of mobile electrons is determined by (1) the density of electrons available for screening, (2) the ratio of electron-ion potential energy to electron kinetic energy, (3) the ratio of a typical electron wavelength to the range of an impurity potential, and (4) the interactions between the screening electrons beyond the Hartree level. If (2) is small, a linear screening model is adequate. When (3) and (4) are negligible, the LTFA model is an accurate approximation to linear screening. When (3) becomes significant, RPA screening is more accurate than LTFA, and when (4) is important, local-field corrections modify the RPA result. All four factors are density and temperature dependent.

Previous calculations of carrier mobility in semiconductors which have combined the LTFA screening model with the Born approximation for electron-impurity scattering cross sections have yielded mobilities that are consistently higher than experimental values, particularly for cases with multiple-valley conduction bands.[20] Meyer and Bartoli have made extensive calculations of carrier mobilities in semiconductors,[1,21] using the phase-shift method to find the electron-impurity scattering rate with the Friedel sum rule to determine the screening length of the impurity potential, which they assumed to be of the LTFA form. Their results show differences between theory and experiment that are smaller than the Born results but still substantial, with the theoretical mobilities for Si at room temperature nearly twice as large as the experimental values for impurity concentrations of $10^{19}-10^{20}$ cm^{-3}. In a study of the reasons for this discrepancy, they have used LTFA and the Born approximation to argue that the conventional linear extrapolation from the problem of free electrons screening a single ion to screening in a multi-ion system is not accurate.[1,22] They found corrections to the conventional treatment which appear to considerably improve the agreement with experiment in the "strong screening limit," where the LTFA screening length q_{TF}^{-1} is much shorter than the average distance between impurities. An important implication of their analysis is that the strong screening regime is unphysical and that neighboring ions must necessarily overlap to some extent.

LTFA is an approximation to RPA, becoming equivalent in the limit of small momentum transfer, q. The work of Saso and Kasuya[23] suggests that LTFA is not reliable for understanding transport when q_{TF}^{-1} is small compared to a scattering electron wavelength. They observed that, at zero temperature, the Fermi wave vector $k_F=(2m^*E_F)^{1/2}/\hbar$ is less than $q_{\mathrm{TF}}/2$ in multiple-valley Ge for a wide range of impurity concentrations, whereas the opposite is true if n_{val} is set equal to unity. They also pointed out that large q values of $\epsilon(q)$ become important and LTFA becomes invalid when $2k_F<q_{\mathrm{TF}}$. At nonzero temperatures, ϵ_{RPA} is less than ϵ_{LTFA} when the impurity potential is not slowly varying compared to the wavelengths of electrons in states for which $-\partial f/\partial E$ is large. The present study shows that this is the case in n-type silicon for conditions close to those under which strong screening is observed, namely in the higher concentration range at 300 K and for a wide range of concentrations at 77 K. Thus, in agreement with Meyer and Bartoli,[1,22] screening is weaker and mobilities are lower in this regime than conventional LTFA predicts. However, in disagreement with them, the RPA result does not imply that impurity ion potentials must always overlap.

Saso and Kasuya[23] found that, at zero temperature, RPA screening reproduced the characteristic features of impurity potentials in Ge obtained by more accurate nonlinear many-body methods. However, the $T=0$ resistivities they obtained with the phase-shift method and the nonlinear Hartree method (a nonlinear version of RPA) were higher than the RPA values. Their inclusion of exchange and correlation contributions resulted in even higher resistivities in good agreement with experiment for doping levels above 3×10^{18} cm^{-3}. On the other hand Chattopadhyay's[24] combination of the Born approximation with a temperature-dependent solution of the nonlinear Poisson equation (a nonlinear version of LTFA) yields resistivities that are lower than the LTFA values, increasing rather than decreasing the discrepancy between theory and experiment.

Temperature-dependent RPA screening was used with the Born approximation for electron-impurity scattering cross sections to calculate resistivities in Ge by Saso and Kasuya,[23,25] who solved the Boltzmann equation, and in Si by Sernelius,[2] who used a memory-function approach. Both studied the effects of anisotropic band structure, concluding that these effects cannot explain the discrepancy between theory and experiment. This paper presents the first calculations of mobility in a doped semiconductor which combine temperature-dependent RPA screening with phase-shift scattering cross sections. Agreement with experiment is better than with the Born RPA, though a discrepancy remains in the lower concentration range. Some understanding of the weaknesses of the model are gained through study of the Freidel and compressibility sum rules.

Section II describes the method used for numerically solving the Boltzmann equation. Section III shows the form of the electron-phonon and electron-impurity scattering rates, and shows how the phase-shift method and the temperature-dependent RPA dielectric function were used. A comparison is made between the Boltzmann-equation solution and the method of Ref. 2 and the calculated mobilities are compared to experiment. Section IV discusses the conditions for validity of linear screening theory, the Born approximation, and the Boltzmann equation in terms of the electron-impurity coupling strength and the Friedel sum rule. Section V shows how the LFC influences the dielectric response and compressibility of the electron gas at nonzero temperatures. Section VI offers some conclusions.

II. SOLUTION OF THE BOLTZMANN EQUATION

The drift mobility is defined as the average drift velocity, $v=\hbar k/m_c^*$, per unit electric field, in the limit of zero electric field. To take the average, the nonequilibrium electron distribution function $F(\mathbf{k})$ can be found from the Boltzmann equation. In steady state under a spatially homogeneous field $\mathcal{E}$,

$$\frac{1}{\Omega}\sum_{\mathbf{k}'}\{W(\mathbf{k},\mathbf{k}')F(\mathbf{k})[1-F(\mathbf{k}')] - W(\mathbf{k}',\mathbf{k})F(\mathbf{k}')[1-F(\mathbf{k})]\}=\frac{-e\mathcal{E}}{\hbar}\cdot\frac{\partial F(\mathbf{k})}{\partial \mathbf{k}}, \tag{3}$$

where $S(\mathbf{k},\mathbf{k}')$ is the probability per unit time that an electron in the initial state $\mathbf{k}$ will make a transition to the final state $\mathbf{k}'$, and Ω is the volume of the system. We have used Rode's method[26] for solving the equation which assumes that the deviation of $F(\mathbf{k})$ from $f(k)$ is small and proportional to the cosine of the angle between $\mathcal{E}$ and $\mathbf{k}$, that is,

$$F(\mathbf{k})=f(k)+f(k)+g(k)\cos\theta\ . \tag{4}$$

It is also assumed that only a small electric field is applied so that $g(k)$ is first order in $\mathcal{E}=|\mathcal{E}|$. Equation (4) is exact only for spherical energy surfaces, but is taken as an ansatz here. Then, the differential scattering rate $W(\mathbf{k},\mathbf{k}')$ depends only on $k=|\mathbf{k}|$, $k'=|\mathbf{k}'|$, and γ, the angle between $\mathbf{k}$ and $\mathbf{k}'$. Using the law of cosines, an exact integral equation for $g(k)$ in terms of $g(k')$ results,[26]

$$\frac{e\mathcal{E}}{\hbar}\frac{\partial f}{\partial k}=\frac{1}{\Omega}\sum_{\mathbf{k}'}g(k')\cos\gamma\{W(\mathbf{k}',\mathbf{k})[1-f(k)] + W(\mathbf{k},\mathbf{k}')f(k)\} -g(k)\frac{1}{\Omega}\sum_{\mathbf{k}'}\{W(\mathbf{k},\mathbf{k}')[1-f(k')] + W(\mathbf{k}',\mathbf{k})f(k')\}\ . \tag{5}$$

No assumption of parabolity is necessary to Rode's method. However, parabolic bands have been assumed throughout the present calculation since the conduction band of silicon is very nearly parabolic near its minima.

The differential scattering rate $W(\mathbf{k},\mathbf{k}')$ is a sum of rates for elastic and inelastic processes, $W(\mathbf{k},\mathbf{k}')=W_{\text{el}}(\mathbf{k},\mathbf{k}')+W_{\text{inel}}(\mathbf{k},\mathbf{k}')$. For elastic processes only, $k=k'$, and a simple "relaxation-time" form results. The dependence of $g(k)$ on $g(k')$ due to inelastic events which scatter electrons *into* the state $\mathbf{k}$ implies that, in general, an iterative solution for $g(k)$ is necessary. However, if the inelastic differential scattering rates do not depend on the angle γ, their contribution to the first sum on the right-hand side of Eq. (5) vanishes. This is the case for doped silicon when electron-electron scattering is ignored as in the present work, since the only remaining inelastic mechanism is intervalley scattering by phonons which is approximately γ independent due to the wide separation between valleys. The only intervalley scattering events whose effect changes in the equilibrium distribution function are those which scatter electrons *out of* the state $\mathbf{k}$. The solution for $g(k)$ to first order in the applied electric field is then

$$g(k)=-\frac{e\mathcal{E}}{\hbar}\frac{\partial f}{\partial k}\left[\frac{1}{\tau_{\text{el}}(k)}+\frac{1}{\tau_{\text{inel}}^{\text{out}}(k)}\right]^{-1}, \tag{6}$$

where

$$\frac{1}{\tau_{\text{el}}(k)}=\frac{1}{\Omega}\sum_{\mathbf{k}'}(1-\cos\gamma)W_{\text{el}}(\mathbf{k},\mathbf{k}') \tag{7}$$

and

$$\frac{1}{\tau_{\text{inel}}^{\text{out}}(k)}=\frac{1}{\Omega}\sum_{\mathbf{k}'}\{W_{\text{inel}}(\mathbf{k},\mathbf{k}')[1-f(k)] + W_{\text{inel}}(\mathbf{k}',\mathbf{k})f(k)\}\ . \tag{8}$$

III. SCATTERING RATES AND MOBILITY

The first approximation to $W(\mathbf{k},\mathbf{k}')$ is the Born approximation, that is, Fermi's golden rule that $W(\mathbf{k},\mathbf{k}')$ is proportional to the square of the matrix element for the interaction potential between the electron and a scattering center. In contrast, the phase-shift method yields an exact result for $W(\mathbf{k},\mathbf{k}')$. Both methods require a model to represent the interaction potentials.

Some previous calculations[27,28] of carrier mobility in silicon have included a constant factor to take into account the fact that electron-electron scattering can distort the electron distribution function and thus change the electron-impurity and electron-phonon scattering rates. However, Appel's work[29] indicates that, for nondegenerate statistics, the correction factor is not constant but depends on the carrier wavelength and the screening length $1/q_{\text{TF}}$, becoming insignificant for the doping range considered here. Meyer and Bartoli[1] used Appel's scattering rates in a variational solution of the Boltzmann equation for isotropic energy surfaces and found that the electron-electron scattering correction at 300 K is never greater than a few percent at any doping level. Therefore, it has been neglected in the present work.

Recently, Fischetti[30] made an approximate calculation of the electron-plasmon scattering rate and found a significant reduction in electron mobility. A more careful study of collective electronic excitations would be of interest, especially with regard to the issue of strong coupling. A negative plasmon dispersion relation is linked to negative electronic compressibility.[13]

Selection rules allow intravalley electron-phonon scattering in Si only by acoustic phonons.[31] This process was treated as elastic and a simple isotropic dilation was assumed. Since k_BT is large compared to the relevant acoustic-phonon energies, Eq. (7) yields, for the scattering rate,

$$\frac{1}{\tau_{\text{ac}}(k)}=\frac{E_1^2k_BTkm^*}{c_l\hbar^3\pi}, \tag{9}$$

where E_1 is the acoustic deformation-potential constant and $c_l=19.07\times10^{10}N/m^2$ is the spherically averaged elastic constant for longitudinal modes. As Rode showed,[32] the contribution from intervalley scattering is of about the same magnitude as intravalley scattering at room temperature in silicon. Because the relaxation-time approximation is not made in Rode's method, the inelastic character of carrier scattering from optical phonons is accurately accounted for. From Eq. (8), the scattering rate for this process is

$$\frac{1}{\tau_{\mathrm{iv}}(k)}=\frac{D^2(n_{\mathrm{val}}-1)m^*}{2\pi\rho\omega\hbar^2}\{k^-[N+1-f(k^-)]+k^+[N+f(k^+)]\}\ , \tag{10}$$

where

$$k^{\pm}=\left[k^2\pm\frac{2m^*}{\hbar}\omega\right]^{1/2} .$$

In this expression, N is the phonon distribution function, D is the deformation-potential constant for intervalley scattering, $\rho=2.33$ g/cm^3 is the mass density of silicon, and $\hbar\omega$ is the phonon energy. Using the temperature dependence of the band gap and electron and hole effective masses compiled by Green,[33] the values for the deformation-potential constants $E_1=9.6$ eV and $D=6.5\times10^8$ eV/cm used in this work were empirically derived by comparison between the measured[34] and calculated temperature dependence of electron mobility in intrinsic silicon. Intervalley scattering of electrons is predominantly by a 58.5-meV transverse-optical phonon, resulting in transitions between perpendicular valleys (f-type scattering).[35,36] Other workers have included minor contributions from as many as five other phonons for intervalley scattering.[37] However, using only the values of E_1 and D stated above yields mobilities which are within 10% of the experimental values of Canali *et al.*[34] for the 70–420-K temperature range. Any variation of these values with doping has been neglected.

Elastic scattering of carriers by ionized impurities has frequently been calculated in the Born approximation with a Coulomb potential screened according to finite-temperature LTFA.[38,39] Solving the linearized Poisson equation in the finite-temperature Thomas-Fermi approximation gives, for the screened potential of an impurity of charge Ze,

$$\phi_{\mathrm{LTFA}}(r)=\frac{Ze}{\epsilon_\infty r}\exp(-q_{\mathrm{TF}}r)\ , \tag{11}$$

where

$$q_{\mathrm{TF}}^2=\frac{4\pi e^2}{\epsilon_\infty}\frac{\partial n}{\partial\mu}=\frac{4\pi e^2}{\epsilon_\infty k_BT}\int_0^\infty N(E)f(E)[1-f(E)]dE \tag{12}$$

is the square of the inverse screening length of the impurity potential. Here μ denotes the chemical potential and $N(E)=n_{\mathrm{val}}m^*k/\pi^2\hbar^2$ is the density of states in energy for both spins. Using Eq. (7) and the Born approximation for scattering from ϕ_{LTFA} yields the Brooks-Herring electron-impurity scattering rate for a concentration of N_i impurities,

$$\frac{1}{\tau_{\mathrm{imp}}^{\mathrm{BH}}(k)}=\left[\frac{Ze^2}{\epsilon_\infty}\right]^2\frac{2\pi m^*}{(\hbar k)^3}N_i\left[\ln(y+1)-\frac{y}{y+1}\right]\ , \tag{13}$$

where

$$y=4k^2/q_{\mathrm{TF}}^2 .$$

Whereas the Born approximation is valid only when the impurity potential does not significantly perturb the scattering electron wave function, the phase-shift cross section is exact.[40] For a spherically symmetric potential, the phase shifts $\delta_l(k)$ for the partial wave of angular momentum l are calculated by numerically solving the radial part of the Schrödinger equation and matching the numerical solution for the wave function in the region where $\phi(r)\rightarrow0$ to the solution with $\phi(r)=0$,

$$R(r)=c[j_l(kr)-\tan\delta_l(k)n_l(kr)] .$$

Here $j_l(kr)$ and $n_l(kr)$ are spherical Bessel and Neumann functions, respectively, and c is a normalization constant. The scattering rate is[41,21]

$$\frac{1}{\tau_{\mathrm{imp}}^{\mathrm{ps}}(k)}=N_i\frac{4\pi\hbar}{km^*}\sum_{l=0}^{\infty}(l+1)\sin^2(\delta_l-\delta_{l+1}) . \tag{14}$$

The Friedel sum rule may be used to find an optimized screening length for ϕ_{LTFA} because it imposes a self-consistency condition requiring that the free-carrier screening charge exactly cancel the ionized impurity charge at large distances. Optimization with the Friedel sum rule is implemented by varying q_{TF} in $\phi_{\mathrm{LTFA}}(r)$ until the phase shifts found by solving the Schrödinger equation satisfy Eq. (1). The present study shows that the optimum screening lengths found with the sum rule are consistently smaller in the semidegenerate regime than LTFA predicts according to Eq. (12).

As was suggested in the introduction, LTFA is probably not a good model for screening when impurity potentials are not slowly varying compared to the scattering electron's wavelength. A more accurate linear screening model is the RPA, which accounts for the dependence of screening on the momentum transfer, q. In this case, the screened electron-ion potential energy is

$$-e\phi_{\mathrm{RPA}}(r)=-\frac{1}{(2\pi)^3}\int d^3q\frac{v_q^\infty}{\epsilon_{\mathrm{RPA}}(q)}\exp(iqr)\ , \tag{15}$$

where $v_q^\infty=4\pi e^2/q^2\epsilon_\infty$. The static RPA dielectric function may be written as

$$\epsilon_{\mathrm{RPA}}(q)=1-v_q^\infty\frac{n_{\mathrm{val}}}{\pi^2}\frac{m^*}{\hbar^2}\int_0^\infty dk\frac{\partial f(k)}{\partial k}kY\left[\frac{q}{2k}\right]\ , \tag{16}$$

where

$$Y(x)=\tfrac{1}{2}+\frac{1}{4x}(1-x^2)\ln\left|\frac{x+1}{x-1}\right| .$$

For small x, $Y(x)$ approaches unity and ϵ_{RPA} approaches $\epsilon_{\mathrm{LTFA}}=1+q_{\mathrm{TF}}^2/q^2$. For large x, $Y(x)$ approaches zero and $\epsilon_{\mathrm{RPA}}<\epsilon_{\mathrm{LTFA}}$. However, both ϵ_{RPA} and ϵ_{LTFA} are close to unity for very large q. Therefore, the difference between RPA and LTFA is only significant when both $q_{\mathrm{TF}}^2\approx q^2$ and $q\gg k$ for relevant k values. This occurs whenever the impurity potential is not slowly varying compared to electron wavelengths in states for which $-\partial f/\partial E$ is large.

For comparison, results are presented here for mobilities calculated with ϵ_{RPA} both with the phase-shift method and with the Born approximation for the scattering rate,

$$\frac{1}{\tau_{\text{imp}}^{\text{Born}}(k)}=\left[\frac{Ze^2}{\epsilon_\infty}\right]^2\frac{4\pi m^*}{(\hbar k)^3}N_i\int_0^{2k}dq\frac{1}{q}\left[\frac{1}{\epsilon(q)}\right]^2 . \qquad (17)$$

The mobility is found with the nonequilibrium distribution function and may be written as

$$\mu_{\text{drift}}=\frac{e}{m_c}\langle\tau\rangle_\mu . \qquad (18)$$

Here, $\tau=(\sum_i 1/\tau_i)^{-1}$, where the index i runs over all scattering mechanisms, and the average $\langle\ \rangle_\mu$ is defined as

$$\langle A\rangle_\mu\equiv\frac{2}{3n}\int N(E)EA(E)\left[-\frac{\partial f}{\partial E}\right]dE . \qquad (19)$$

Since the scattering rates are added before the average is taken, Matthiessen's rule has not been invoked. It should be pointed out that the mobility obtained by solving the Boltzmann equation may differ from the mobility obtained with the "generalized Drude approach" (GDA) used in Ref. 2. The latter method is also known as the memory-function[42] or force-force correlation function[43] approach. It yields an approximate result for the conductivity for arbitrary frequency of the applied field. The GDA mobility is determined from the zero-frequency limit of the imaginary part of the memory function.[42] For the case of elastic scattering from impurities,

$$\mu_{\text{drift}}^{\text{GDA}}=\frac{e}{m_c}\left\{\lim_{\omega\to 0}\frac{2N_i}{3n^2}\frac{\omega_p^2}{\omega}\int\frac{d^3q}{(2\pi)^3}\text{Im}[\epsilon^{-1}(q,0)-\epsilon^{-1}(q,\omega)]\right\}^{-1} ,$$

where $\omega_p^2=4\pi e^2 n/\epsilon_\infty m^*$. It can be shown that, using the RPA dielectric function ϵ_{RPA},

$$\mu_{\text{drift}}^{\text{GDA}}=\frac{e}{m_c}\frac{1}{\langle 1/\tau\rangle_\mu} , \qquad (20)$$

where $1/\tau(E)$ is determined in the Born approximation, as in Eq. (17). After making the isotropic approximation used here, Eqs. (3.16) and (3.17) of Ref. 2 become equal to $\langle 1/\tau\rangle_\mu$. The GDA result for the resistivity due to impurity scattering is equivalent to the lowest order variational solution to the linearized Boltzmann equation,[44] in which one assumes as trial function $g(k)=-(\alpha e\mathcal{E}/\hbar)\partial f/\partial k$. The variational principle determines the optimum value of α to be $\langle 1/\tau\rangle^{-1}$. At nonzero temperatures, $\langle 1/\tau\rangle_\mu$ is greater than $1/\langle\tau\rangle_\mu$, though they become equal in the degenerate limit. The ratio of $1/\langle\tau\rangle_\mu$ to $\langle 1/\tau\rangle_\mu$ is easily shown to be $3\pi/32\approx 0.29$ in the classical limit,[45] assuming an energy dependence $\tau(E)\propto E^{3/2}$. Figure 1 is similar to Fig. 1 of Ref. 2 and shows a comparison of the GDA and Boltzmann-equation solutions for the temperature dependence of the electrical resistivity of Si due to impurity scattering only. It is evident that significant differences arise between the two solutions in systems away from the degenerate limit. A similar observation was made by Lai and Ting[46] for a two-dimensional semiconductor system. The more accurate result is the one obtained by solving the Boltzmann equation. The Kubo formula, which is the exact result for the linear response to an applied field, reduces to the linearized Boltzmann-equation result in the weak-coupling limit for the case of elastic scattering.[47,48] The full (nonlinearized) Boltzmann equation for electron-impurity scattering can be rigorously derived in the same limit with the Keldysh formalism.[49] The "weak-coupling" criterion and the range of validity of the Boltzmann equation are discussed in the next section.

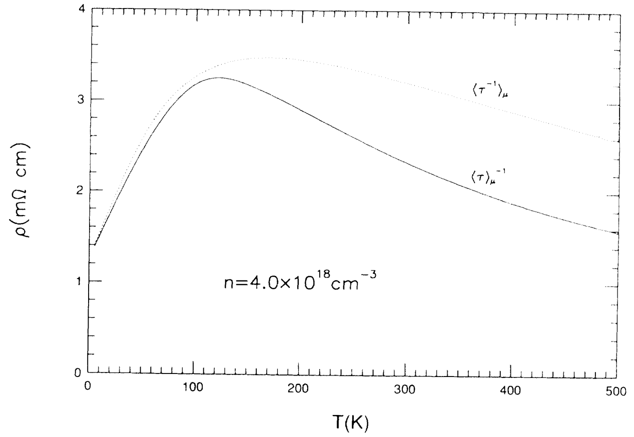

FIG. 1. Electrical resistivity vs temperature in silicon for impurity scattering only. The donor concentration is 4×10^{18} cm^{-3}. The upper curve is the GDA result and the lower curve is the Boltzmann equation result in the RPA Born approximation.

Figures 2 and 3 show the calculated donor concentration dependence of electron mobility in silicon at 300 and 77 K compared to experiments[50,51] on phosphorus-doped samples. A few points are immediately noticeable. (1) The phase-shift method yields electron mobilities in n-type silicon that are consistently lower than those obtained in the Born approximation. (2) Mobilities calculated with LTFA screening and phase-shift cross sections are higher when the screening length is optimized with the Friedel sum rule. Thus satisfaction of the rule does not improve agreement with experiment for this case. (3) RPA yields mobilities that are significantly lower than the LTFA values for all densities at 77 K and in the higher concentration range at 300 K. (4) At both temperatures, the RPA phase shift results are higher than the experimental values in the lower concentration range, while agreement appears to be rather good at the high end. The experiments determined donor concentration from Hall measurements, assuming that the ratio of Hall to drift mobilities is unity at room temperature. There is evidence[52] that this ratio differs from unity in the $10^{17}-10^{19}$ cm^{-3} concentration range and can be as high as 1.3 at 10^{18} cm^{-3}.

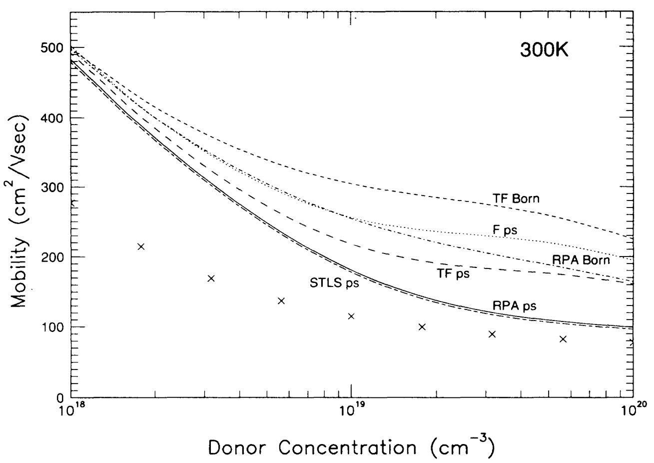

FIG. 2. Electron mobility in n-type silicon at 300 K. The calculated curves are labeled as follows. TF: LTFA screening; RPA: RPA screening; F: LTFA screening optimized with the Friedel sum rule; STLS: screening with $\Lambda/\epsilon_{\text{STLS}}$; Born: Born approximation cross section; ps: phase-shift cross section. Values from the computer fit to experiment by Masetti, Severi, and Solmi (Ref. 50) are indicated by ×.

IV. LINEAR SCREENING AND THE FRIEDEL SUM RULE

In this section it is shown that, for fixed nonzero temperature, the dimensionless Coulomb coupling constant of an interacting electron gas is nonmonotonic in density and that, whenever it is large, the LTFA and RPA theories predict that the electron-ion interaction is strong. In this case, linear screening theory, the Born approximation for the electron-ion scattering rate, and the electron-impurity Boltzmann equation are all questionable. Strong violations of the Friedel sum rule can be interpreted as a signal of the breakdown of perturbation theory in the electron-ion coupling on which all three approximations are based.

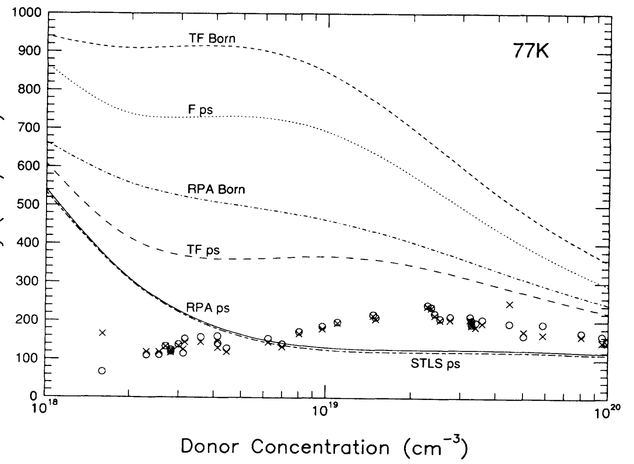

FIG. 3. Electron mobility in n-type silicon at 77 K. Calculated curves are labeled as in Fig. 1. The experimental values of Yamanouchi, Mizuguchi, and Sasaki (Ref. 51) are indicated by × (R_H/ρ) and ○ ($1/ne\rho$).

The dimensionless measure of the importance of electron-electron coupling in an interacting electron gas is the ratio of Coulomb to kinetic energies.[53] In the classical limit of high temperature and low electron density, this ratio is

$$\left[\frac{e^2}{\epsilon_\infty a}\right] \Big/ \left(\tfrac{3}{2}k_B T\right) = \tfrac{2}{3}\Gamma ,$$

where $a=(3/4\pi n)^{1/3}$ is the radius of a sphere of volume $1/n$, referred to as the Wigner-Seitz radius. When quantum effects are important as in a degenerate doped semiconductor, the kinetic energy is measured by E_F and the energy ratio is

$$\frac{e^2}{\epsilon_\infty a E_F} = r_s' = 2\left[\frac{4n_{\text{val}}}{9\pi}\right]^{2/3} r_s ,$$

where $r_s=a/a_B$, and $a_B=\hbar^2\epsilon_\infty/m^* e^2$. Notice that Γ *increases* with density, whereas r_s *decreases* with density. In passing from the classical to the degenerate limit, the electron-electron coupling strength is not a monotonic function of density. The expressions for the classical and degenerate limits are equal at $k_B T=2/3E_F$. Thus, viewed as a function of density for constant temperature, the coupling strength is expected to have a maximum near $\Theta=\frac{2}{3}$. A function which describes the electron-electron coupling strength for arbitrary degree of degeneracy is

$$C_{\text{ee}} = \frac{e^2}{\epsilon_\infty a \langle KE \rangle} , \tag{21}$$

where

$$\langle KE \rangle = \frac{\int_0^\infty E\left[-\frac{\partial f}{\partial E}\right] N(E)dE}{\int_0^\infty \left[-\frac{\partial f}{\partial E}\right] N(E)dE} = \frac{6\pi e^2}{\epsilon_\infty}\frac{n}{q_{\text{TF}}^2} . \tag{22}$$

The last form for $\langle KE \rangle$ follows from Eq. (12). Dandrea, Ashcroft, and Carlsson[19] have proposed a similar functional form for the coupling strength of an electron gas of arbitrary degeneracy. However, they chose for $\langle KE \rangle$ an average over the entire electron distribution function, $f(E)$, rather than only over the part describing electrons available for interactions, $-\partial f/\partial E$. Therefore, their expression differs in the degenerate limit.

The function C_{ee} together with its degenerate and classical limits is plotted in Fig. 4 for 300 and 77 K. The plot shows that $C_{\text{ee}} > 1$ for heavily doped silicon at 300 K and for a broad range of concentrations at 77 K, indicating that the electron-electron interactions cannot be considered weak in these regions.

The electron-electron coupling strength defined above may be written as

$$C_{\text{ee}} = \tfrac{2}{9} q_{\text{TF}}^2 a^2 , \tag{23}$$

an exact relation for arbitrary degeneracy, showing that strong electron-electron coupling implies q_{TF}^{-1} small compared to a, equivalent to strong screening in the LTFA. This is the "dilute-gas limit," but does not correspond to

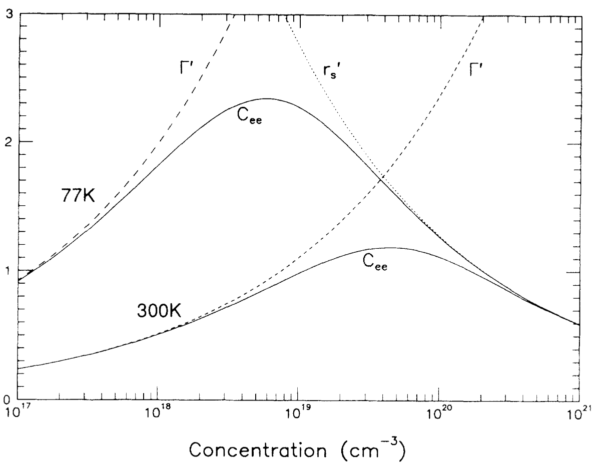

FIG. 4. Electron-electron coupling constant C_{ee} vs electron concentration for 300 and 77 K. Also shown are $r_s' = 2(8/3\pi)^{2/3} r_s$ and $\Gamma' = 2/3\Gamma$ at the two temperatures.

the lowest impurity concentrations since q_{TF}^{-1} increases rapidly with decreasing density as the system moves toward nondegeneracy. In the extreme degenerate and nondegenerate limits, $q_{\text{TF}}^{-1} \approx a$ and impurities should be thought of as overlapping. However, for doped silicon in the semidegenerate regime, this is not the case.

To define a convenient dimensionless measure of the electron-ion coupling strength, C_{ei}, one can choose the LTFA impurity potential $\phi_{\text{LTFA}}(r)$ evaluated at q_{TF}^{-1} to represent the electron-ion potential energy. Then, for $Z=1$,

$$C_{\text{ei}} = \frac{\frac{e^2}{\epsilon_\infty} q_{\text{TF}} \exp(-1)}{\langle KE \rangle} . \tag{24}$$

When C_{ee} is large, C_{ei} is large as well. Comparison of Eqs. (21), (23), and (24) shows that $C_{\text{ei}} = 0.78 C_{\text{ee}}^{3/2}$. In the strong screening limit, electrons and impurities are most strongly interacting. Since $\epsilon_{\text{RPA}}(q) \le \epsilon_{\text{LTFA}}(q)$, impurities are screened less and the electron-impurity coupling is stronger in the RPA than in the LTFA for the same value of C_{ee}. The difference should be greatest when q_{TF}/k is large for interacting electrons, since then the RPA differs most from the LTFA. It is shown next that C_{ei} is the Thomas-Fermi measure of validity of linear-response theory for screening of impurities by electrons and for scattering of electrons by impurities.

The Thomas-Fermi expression for the electron density in the presence of ϕ_{ext} has the same functional form as for the unperturbed density, but with the chemical potential μ shifted by $e\phi(r)$. The screening density is then $\delta n(r) = n[\mu + e\phi(r)/k_B T] - n(\mu/k_B T)$. In the LTFA, δn is calculated by Taylor expanding the perturbed density and retaining only the linear term. Using Eq. (22) to write $C_{\text{ei}} = q_{\text{TF}}^3 \exp(-1)/6\pi n$ shows that a small C_{ei} implies a small linear term compared to the unperturbed density, that is, $e\phi \partial n/\partial \mu = q_{\text{TF}}^3 \exp(-1)/4\pi \ll n$. At 77 K, the linear screening density is actually *larger* than the unperturbed density from 5×10^{17} to 5×10^{19} cm^{-3}, indicating that linear screening theory is not reliable in this range. In a study of the nonlinear Poisson equation in the Thomas-Fermi approximation, Meyer[54] established a similar criterion that if the quadratic term is small compared to the linear one, the linear screening approximation is adequate. Both criteria require that the electron-impurity potential energy be weak in comparison to a characteristic electron energy in order for the linear theory to be valid.

The Born cross section is also a first-order approximation. Figure 5 shows the concentration dependence of μ_B/μ_{ps}, the ratio of Born to phase shift mobilities for 300 and 77 K in the LTFA and RPA. The Born results approach the phase-shift results in the most nondegenerate regime studied, low densities at 300 K. In this limit one finds also from Fig. 5 that $(q_{\text{TF}}/\bar{k})^2 \equiv \hbar^2 q_{\text{TF}}^2 / 2m^* \langle KE \rangle$ is small, consistent with the fact that the Born approximation is valid for high-energy scattering electrons. In the semidegenerate regime $(q_{\text{TF}}/\bar{k})^2$ is generally not small for silicon. From the definition of C_{ei},

$$\frac{\hbar^2}{2m^*} \frac{q_{\text{TF}}^2}{\langle KE \rangle} = C_{\text{ei}} \frac{q_{\text{TF}} a_B}{2\exp(-1)} . \tag{25}$$

Since $q_{\text{TF}} a_B \sim 1$ when C_{ei} is maximum, $(q_{\text{TF}}/\bar{k})^2$ cannot be small unless C_{ei} is small.

For low-energy scattering from the LTFA potential, the criterion for the validity of the Born approximation is $2/a_B q_{\text{TF}} \ll 1$,[55] roughly the condition that the screened potential not be attractive enough to form a bound state. Equation (25) shows that if $2/a_B q_{\text{TF}} \ll 1$, then C_{ei} cannot be very large, even if $(q_{\text{TF}}/\bar{k})^2 > 1$. Therefore, in this case also, the Born approximation cannot be valid if C_{ei} is large. Figure 5 shows that the Born results differ significantly from the phase-shift results at 77 K. As expected, μ_B/μ_{ps} is greater for the RPA than for the LTFA when $q_{\text{TF}}/2\bar{k}$ is large.

If the Born approximation for the phase shifts is valid, the LTFA ion potential exactly satisfies the Friedel sum

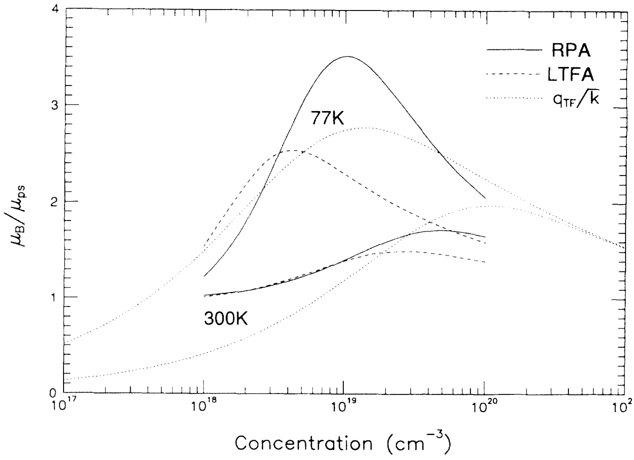

FIG. 5. Ratio of Born to phase-shift electron mobilities for n-type silicon calculated in the RPA and in the LTFA. The upper set of curves is for 77 K and the lower set is for 300 K. For comparison, $q_{\text{TF}}/\bar{k}$ is indicated by the dotted lines.

rule.[56,6] The right-hand side of Eq. (1) is plotted in Fig. 6 as a function of concentration for 300 and 77 K. If the rule was perfectly satisfied, the curves would have a constant value of unity. The strongest violation of the sum rule does not necessarily occur precisely where C_{ei} is maximum. In all cases studied, it occurs when the impurity potential is just strong enough to form its first bound state. As the density is decreased for fixed temperature, more bound states develop, but the sum rule becomes increasingly well satisfied as $q_{\text{TF}}a$ becomes small. These facts indicate that in order for the rule to be strongly violated, $q_{\text{TF}}a$ must be large and the potential must be strong enough to form a bound state. This is in accord with Friedel's observation that, for a strong and localized perturbing potential, the rigid band model for the energy spectrum of an alloy or a doped semiconductor fails near a band edge since bound states are formed there from extended states.[56] In this case, doping is not well described by a small, rigid shift in energy of the whole curve of the density of states, because the bound-state energies vary much more rapidly with the perturbation than do those of the extended states.

The criterion that C_{ei} be small in order for linear screening theory to be valid is derived from the Thomas-Fermi theory, which breaks down when $\phi(r)$ is not slowly varying compared to the scattering electron wavelength. It does not account for the polarization of the screening electrons by the colliding electron and hence is not as accurate as the RPA for the large-angle scattering characteristic of potentials that are short range in comparison to the scattering electron's wavelength.[57] Linear screening can be valid when the Thomas-Fermi theory is not. This explains why RPA gives better results when $q_{\text{TF}}/\bar{k}$ is large and the potential is not strong enough to form a bound state. On the other hand, the strong violations of the Freidel sum rule by the RPA screened potentials in the $10^{18}-10^{19}$-cm^{-3} range at 77 K are a signal that linear screening theory is not valid under these conditions.

The criterion for the validity of the Boltzmann equation for transport in normal metals is usually stated as $\hbar/\tau(E_F) \ll E_F$ or $k_F l \gg 1$, where l denotes the mean free path of the electron.[58] Chester and Thellung[47] showed that, when this criterion is satisfied, the Boltzmann equation for elastic scattering is an accurate approximation to the exact Kubo formula for the electrical conductivity of a metal. Their method was to expand the conductivity in powers of λ, where λ measures the strength of the scattering potential. They found that the higher-order terms are negligible when $\hbar/\tau \ll E_F$. In the present discussion, C_{ei} plays the role of λ. A natural generalization of the validity criterion for arbitrary degeneracy is

$$\frac{\hbar}{\langle \tau \rangle_\mu} \ll \langle KE \rangle \ , \tag{26}$$

where $\langle \tau \rangle_\mu$ is as defined in Eq. (19). Figure 7 shows that the criterion is not well satisfied when C_{ee}, and consequently C_{ei}, are large. (See Fig. 4.) When inequality (26) is violated, the momentum $\hbar k$ can no longer be considered a good quantum number, the scattering events being too frequent for it to become well defined between them. This breakdown of the description in terms of electrons undergoing independent scattering events is due to the fact that the electron's de Broglie wavelength is long relative to the spacing between impurity potentials. Recalling that $C_{\text{ei}} \propto (q_{\text{TF}}a)^3$, it is clear that the condition is violated when the screening length is small compared to the spacing between impurities, *not* when the impurity potentials are closer to overlapping. A similar conclusion was reached by Meyer and Bartoli[59] on the basis of the equivalent criterion $\tau_D/\tau_R \ll 1$, where τ_D is the duration of the collision and τ_R is the relaxation time.

If $q_{\text{TF}}a \ll 1$, one expects again a breakdown of the picture of quasiparticles with well-defined momentum scattering from one ion potential at a time, since in this case the ions overlap. An intuitively clear criterion which includes both types of breakdown has been proposed:[59]

$$\left[\frac{1}{2q_{\text{TF}}a}\right]^3 + \left[\frac{1}{ka}\right]^3 \lesssim 1 \ . \tag{27}$$

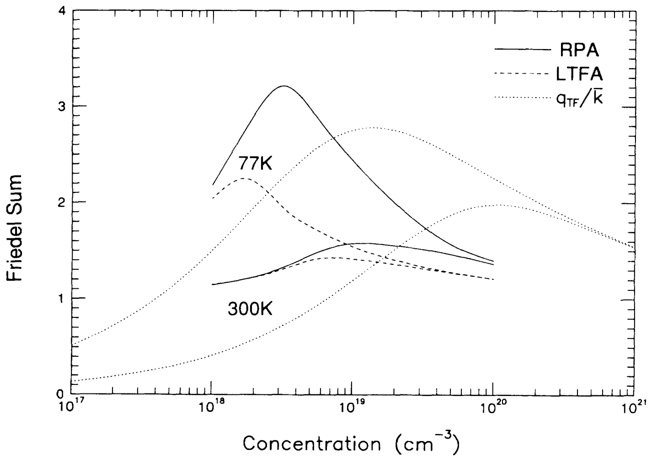

FIG. 6. Friedel sum vs concentration. The set of curves which are upper at the left side are for 77 K and the lower set is for 300 K. For comparison, $q_{\text{TF}}/\bar{k}$ is indicated by the dotted lines.

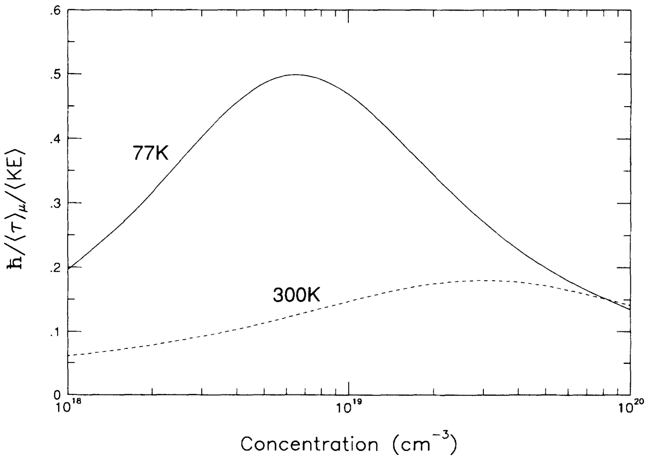

FIG. 7. Validity criterion for the Boltzmann equation. $1/\langle \tau \rangle_\mu$ is an average RPA phase-shift relaxation time as defined in Eq. (19). $\langle KE \rangle$ is as defined in Eq. (22).

Setting $k=\bar{k}$ and using the definition of C_{ei}, this expression can be rewritten as

$$\frac{0.01}{C_{\text{ei}}}+0.45\left[\frac{a_B}{a}\right]^{3/2}C_{\text{ei}}\lesssim 1\ . \tag{28}$$

The highest value of C_{ei} of the cases considered in the present work is 2.8 for a concentration of 6×10^{18} cm^{-3} at 77 K. The second term on the left-hand side of (28) then has the value of 0.52, suggesting that the validity of the Boltzmann equation is becoming questionable in this situation, despite the apparently good agreement with experimental results shown in Fig. 3. Inequality (27) does not explain why agreement with experiment is poor for the lower concentration range at 300 K where C_{ei} and $(q_{\text{TF}}/\bar{k})^2$ are small. At 10^{18} cm^{-3}, $q_{\text{TF}}a=1.5$ and $C_{\text{ei}}=0.28$, making the left-hand side of (28) very small. It appears that the discrepancy in this range cannot be explained in terms of a breakdown of the theory due to strong coupling, and random potential fluctuations associated with overlapping impurity potentials appear irrelevant. However, a criterion for well-defined quasiparticle momenta derived from an energy spectrum analysis more sophisticated than the rigid band model used here might show a violation in this region.

V. LOCAL-FIELD CORRECTION AND COMPRESSIBILITY

The RPA dielectric function accounts for electron-electron interactions only via the Coulomb potential of the average charge density. Beginning with Hubbard,[60] generalizations of the RPA have represented short-range effects as a local-field correction to the average field. In the approximation of a static LFC, $G(q)$, the frequency-dependent dielectric function, ϵ_{LFC}, for a multiple-valley semiconductor is

$$\epsilon_{\text{LFC}}(q,\omega)=1-\frac{n_{\text{val}}v_q^{\infty}P^{(1)}(q,\omega)}{1+v_q^{\infty}G(q)P^{(1)}(q,\omega)}\ , \tag{29}$$

where

$$P^{(1)}(q,\omega)=\frac{2}{(2\pi)^3}\int d^3k\frac{f(E_{\mathbf{k}})-f(E_{\mathbf{k+q}})}{E_{\mathbf{k}}-E_{\mathbf{k+q}}+\hbar\omega+i\delta}$$

is the noninteracting electron polarizability. Singwi *et al.*[3] developed a method for including exchange and correlation effects by expressing $G(q)$ as a functional of the static structure factor $S(q)$,

$$G(q)=-\frac{1}{n}\int\frac{d^3q'}{(2\pi)^3}\frac{(-\mathbf{q}\cdot\mathbf{q}')}{q'^2}[S(\mathbf{q}+\mathbf{q}')-1]\ . \tag{30}$$

Using the fluctuating-dissipation theorem to relate $S(q)$ and $\epsilon(q,\omega)$, they iteratively solved three coupled equations to find ϵ_{LFC} at $T=0$. Tanaka, Mitake, and Ichimaru[4] generalized the method to nonzero temperatures. In this case, the relation between S and ϵ is

$$S(q)+N\delta_{q,0}=-\frac{\hbar}{nv_q^{\infty}}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{1-e^{-\beta\hbar\omega}}\text{Im}\left[\frac{1}{\epsilon(q,\omega)}\right]\ , \tag{31}$$

The fast converging method presented in Ref. 4 was used in the work presented here to solve Eqs. (29)–(31).

Though ϵ_{LFC} can differ dramatically from ϵ_{RPA} when the electron-electron interaction is strong, the local-field correction does not have a large effect on the electron-impurity interaction for the following reason. An electron scattering from an impurity interacts with the screened potential $v_q^{\infty}(\rho_{\text{ext}}+\delta\rho)=\phi_{\text{ext}}/\epsilon(q)$ *plus* an exchange-correlation potential $\phi_{\text{xc}}(q)$ due to its interactions with the other electrons.[61] Therefore, the cross sections and mobility are determined by the electron-test charge interaction potential ϕ_{et} rather than the test charge-test charge interaction potential $\phi_{\text{tt}}=\phi_{\text{ext}}/\epsilon$,

$$\phi_{\text{et}}(q)=\phi_{\text{ext}}(q)/\epsilon(q)+\phi_{\text{xc}}(q)=\phi_{\text{ext}}(q)\frac{\Lambda(q)}{\epsilon(q)}\ , \tag{32}$$

where

$$\Lambda(q)=[1+v_q^{\infty}G(q)P^{(1)}(q)]^{-1}\ .$$

In the RPA, the local-field factor $G=0$ and therefore the vertex function $\Lambda(q)$ is equal to unity. The results of the present study show that values of $\Lambda/\epsilon_{\text{STLS}}$ are similar to those of $1/\epsilon_{\text{RPA}}$, leading to only slight modifications of mobilities[62] as seen in Figs. 2 and 3.

Nevertheless, the dielectric function ϵ_{LFC} itself differs significantly from ϵ_{RPA} when the electron-electron coupling is strong, reflecting changes in important properties of the system when the interaction is turned on. As was shown in the last section, the coupling is strongly temperature and density dependent. The weak-coupling RPA is exact in the high-density limit for the degenerate electron gas, but in the *low-density* limit for the nondegenerate case. In the intermediate regime, ϵ_{RPA} is not accurate.

The RPA gives the noninteracting electron value of the isothermal compressibility $K_{\text{free}}=q_{\text{TF}}^2\epsilon_{\infty}/4\pi e^2n^2$. Figure 8 shows the ratio of the noninteracting gas compressibility K_{free} to K for 300 and 77 K. Taking the $q\rightarrow0$ limit of $\epsilon_{\text{LFC}}(q,0)$ and comparing to Eq. (2) shows that the ratio is

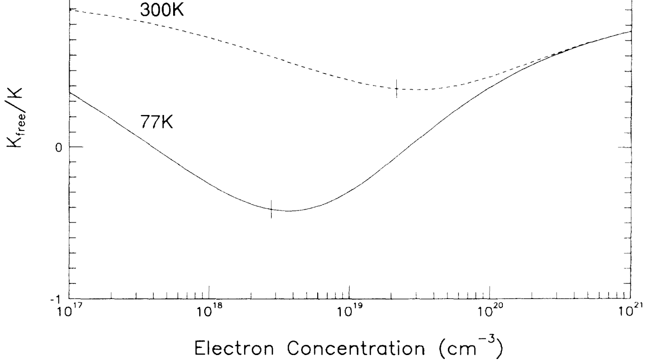

FIG. 8. Ratio of noninteracting to interacting electron-gas compressibilities vs concentration. The vertical lines on the curves are at $\Theta=1$.

$$\frac{K_{\text{free}}}{K}=1-\gamma\left[\frac{q_{\text{TF}}^2}{k_F^2}\right], \tag{33}$$

where

$$\gamma=-\frac{1}{2k_F n_{\text{val}}}\int_0^\infty dq[S(q)-1] \tag{34}$$

is a measure of the electron-electron interaction energy per particle,

$$E_{\text{int}}=\frac{-2n_{\text{val}}}{\pi}\frac{e^2}{\epsilon_\infty}k_F\gamma . \tag{35}$$

Comparison of Eqs. (33) and (35) with Eq. (22) for the average kinetic energy of interacting electrons shows that

$$\frac{K_{\text{free}}}{K}=1+\frac{E_{\text{int}}}{\langle KE\rangle} . \tag{36}$$

Therefore, K_{free}/K is minimum when $-E_{\text{int}}/\langle KE\rangle$ is maximum.

The critical condition for diverging compressibility is

$$E_{\text{int}}^{\text{crit}}=-\langle KE\rangle . \tag{37}$$

Figure 8 shows the result that $K_{\text{free}}/K<0$ for a broad range of electron densities at 77 K in n-type silicon. These results are not unlike those found in the classical and degenerate limits of the electron-gas problem scaled so that $m^*=\epsilon_\infty=n_{\text{val}}=1$. For the zero crossing at lower density, we find that the critical coupling value lies at $\Gamma=2.2$ between the STLS value of $\Gamma=1.3$ found by Berggren[11] and the Monte Carlo value of $\Gamma=3$ found by Hansen.[13] For the upper crossing, we find a critical coupling of $r_s=1.1$, smaller than either the STLS (Ref. 3) value of $r_s=3$ or the Monte Carlo value of $r_s=5.4$ found by Ceperley.[10] Except for the fact that the zero crossings observed for silicon at 77 K occur when the system is not quite in the classical or degenerate limits, the difference between our results and the previous STLS calculations is due to the n_{val} factor, the only nonsimple scaling parameter in the problem.

Negative values for the total compressibility of a system signal an instability.[63] However, two qualifying remarks should be made here. First, the free energy of the system may be found through a coupling-constant integration over the interaction energy.[4] Consistency requires that the second derivative of the free energy with respect to volume give the same answer for the compressibility as obtained with Eq. (2). For $T=0$, Vashishta and Singwi[64] found that K_{free}/K becomes negative at lower electronic densities with the free-energy method until they introduced an improved LFC. Second, even if the two methods give the same result of negative electronic compressibilities, it should not be concluded that an instability could take place in an ordinary bulk-doped semiconductor. When the contribution of the neutralizing background is properly included, the total compressibility may not be negative.[13,53] The local electric field created by a density fluctuation prevents it from building up indefinitely.[13] Nevertheless, the negative K values do indicate that the model used for the study of transport properties may be inadequate to describe the real system for low temperatures and densities. In the previous section it was shown that strong electron-electron coupling can imply an even stronger electron-ion coupling in linear screening theory. In the presence of ionized impurities the strong-coupling electrons should prefer to occupy the bound impurity states than to spontaneously compress to a liquid state. This suggests that the assumption used throughout the calculations presented here, that all impurities are ionized, is not valid. However, there is experimental evidence[65] that free-electron densities at 77 K in doped silicon are nearly the same as at room temperature for this impurity concentration range.

VI. CONCLUSION

Combination of phase-shift cross sections with RPA dielectric screening of impurity potentials yields calculated electron mobilities for n-type silicon that agree with experiment better than LTFA phase-shift or RPA-Born results do. Inclusion of exchange and correlation effects through the finite-temperature STLS dielectric function does not alter the electron interaction with RPA screened impurity potentials by much. A significant discrepancy between theory and experiment persists near 10^{18} for both 300 and 77 K. An examination of the conditions for validity of linear screening theory has shown that the largest discrepancies with experiment occur at lower concentrations than where the theory appears to be most questionable. This fact suggests that simply revising the present model to incorporate nonlinear screening will not eliminate the disagreement with experiment. Improvements over the approximate deformation-potential treatment of electron-phonon scattering used here would certainly be worthwhile, especially at 300 K in the lower impurity concentration range. However, the disagreement with experiment is not well explained by inaccuracies in accounting for electron-phonon effects, since phonons have a negligible influence compared to impurities at 77 K.

In the light of Friedel's remark[56] that the rigid-band model fails near the formation of bound states, it is likely that a more realistic density of states for doped silicon would alter the mobility results. In fact, calculations by Serre and Ghazali[66] and Lowney[67] show that the density of states of doped silicon is significantly altered from the simple model used here, particularly at and below the dopant concentration where the first bound state forms. Also, their analyses of the spectral density of the electron states under these conditions show that momentum is not a good quantum number near the conduction-band edge. Therefore, electrons in these states should have lower mobilities than the values obtained with the Boltzmann equation and the unperturbed dispersion relation. It would be very interesting to see an application of a realistic density of states to a study of transport properties for doped silicon.

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[1] J. R. Meyer and F. J. Bartoli, Phys. Rev. B **36**, 5989 (1987).

[2] B. E. Sernelius, Phys. Rev. B **41**, 3060 (1990).

[3] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).

[4] S. Tanaka, S. Mitake, and S. Ichimaru, Phys. Rev. A **32**, 1896 (1985).

[5] J. Friedel, Nuovo Cimento Suppl. **7**, 287 (1958).

[6] F. Stern, Phys. Rev. **158**, 697 (1967).

[7] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Addison-Wesley, Redwood City, CA, 1989), Vol. I, p. 209.

[8] G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1990), p. 466.

[9] K. Utsumi and S. Ichimaru, Phys. Rev. B **24**, 3220 (1981).

[10] D. Ceperley, Phys. Rev. B **18**, 3126 (1978).

[11] K.-F. Berggren, Phys. Rev. A **1**, 1783 (1970).

[12] H. Totsuji and S. Ichimaru, Prog. Theor. Phys. **52**, 42 (1974).

[13] P. Vieillefosse and J. P. Hansen, Phys. Rev. A **12**, 1106 (1975); J. P. Hansen, *ibid.* **8**, 3096 (1973).

[14] J. P. Eisenstein, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **68**, 674 (1992).

[15] B. Tanatar and D. M. Ceperley, Phys. Rev. B **39**, 5005 (1989).

[16] M. Jonson, J. Phys. C **9**, 3055 (1976).

[17] S. Tanaka and S. Ichimaru, Phys. Rev. B **39**, 1036 (1989).

[18] H. F. Hess, K. DeConde, T. F. Rosenbaum, and G. A. Thomas, Phys. Rev. B **25**, 5578 (1982).

[19] R. G. Dandrea, N. W. Ashcroft, and A. E. Carlsson, Phys. Rev. B **34**, 2097 (1986).

[20] For a review, see D. Chattopadhyay and H. J. Queisser, Rev. Mod. Phys. **53**, 745 (1981).

[21] J. R. Meyer and F. J. Bartoli, Phys. Rev. B **23**, 5413 (1981).

[22] J. R. Meyer and F. J. Bartoli, Phys. Rev. Lett. **57**, 2568 (1986).

[23] T. Saso and T. Kasuya, J. Phys. Soc. Jpn. **48**, 1566 (1980).

[24] D. Chattopadhyay, Phys. Rev. B **23**, 1847 (1981).

[25] T. Saso and T. Kasuya, J. Phys. Soc. Jpn. **49**, 578 (1980).

[26] D. L. Rode, in *Semiconductors and Semimetals,* edited by R. K. Willardson and A. C. Beer (Academic, New York, 1975), Vol. 10, Chap. 1.

[27] S. S. Li and W. R. Thurber, Solid-State Electron. **20**, 609 (1977).

[28] H. S. Bennett, Solid-State Electron. **26**, 1157 (1983).

[29] J. Appel. Phys. Rev. **125**, 1815 (1962); **122**, 1760 (1961).

[30] M. V. Fischetti, Phys. Rev. B **44**, 5527 (1991).

[31] W. A. Harrison, Phys. Rev. **104**, 1281 (1956).

[32] D. L. Rode, Phys. Status Solidi **53**, 245 (1972).

[33] M. A. Green, J. Appl. Phys. **67**, 2944 (1990).

[34] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, and A. Alberigi-Quaranta, Phys. Rev. B **12**, 2265 (1975).

[35] J. G. Nash and J. W. Holm-Kennedy, Phys. Rev. B **15**, 3994 (1977).

[36] J. C. Portal, L. Eaves, S. Askenazy, and R. A. Stradling, Solid State Commun. **14**, 1241 (1974); L. Eaves, R. A. Stradling, J. C. Portal, S. Askenazy, R. Barbaste, and K. Hansen, *ibid.* **15**, 1281 (1974).

[37] R. Brunetti, C. Jacoboni, F. Nava, L. Reggiani, G. Bosman, and R. J. J. Zijlstra, J. Appl. Phys. **52**, 6713 (1981), and references therein.

[38] R. B. Dingle, Philos. Mag. **46**, 831 (1955).

[39] H. Brooks, Phys. Rev. **83**, 879 (1951).

[40] L. I. Schiff, *Quantum Mechanics,* 3rd ed. (McGraw-Hill, New York, 1968).

[41] K. Huang, Proc. Phys. Soc. London **60**, 161 (1948).

[42] W. Götze and P. Wölfle, Phys. Rev. B **6**, 1226 (1972).

[43] See Ref. 8, Secs. 7.3 and 8.1.

[44] J. M. Ziman, *Electrons and Phonons* (Clarendon, Oxford, 1969), pp. 283–285.

[45] M. Huberman and G. V. Chester, Adv. Phys. **24**, 489 (1975).

[46] W. Y. Lai and C. S. Ting, Phys. Rev. B **24**, 7206 (1981).

[47] G. V. Chester and A. Thellung, Proc. R. Soc. London **73**, 745 (1959).

[48] S. F. Edwards, Philos. Mag. **3**, 1020 (1958); J. S. Langer, Phys. Rev. B **120**, 714 (1960).

[49] H. Smith and H. H. Jensen, *Transport Phenomena* (Clarendon, Oxford, 1989), Sec. 8.1.

[50] G. Masetti, M. Severi, and S. Solmi, IEEE Trans. Electron Devices **30**, 764 (1983).

[51] C. Yamanouchi, K. Mizuguchi, and W. Sasaki, J. Phys. Soc. Jpn. **22**, 859 (1967).

[52] F. Mousty, P. Ostoja, and L. Passari, J. Appl. Phys. **45**, 4576 (1974).

[53] S. Ichimaru, Rev. Mod. Phys. **54**, 1017 (1982). This reference gives a value for the classical coupling constant that is $\frac{3}{2}$ times the value used in the present work.

[54] J. R. Meyer, Phys. Rev. B **20**, 1762 (1979).

[55] L. I. Schiff, *Quantum Mechanics* (Ref. 40), p. 326.

[56] J. Friedel, Adv. Phys. **3**, 446 (1954).

[57] N. Takimoto, J. Phys. Soc. Jpn. **14**, 1142 (1959).

[58] H. Smith and H. H. Jensen, *Transport Phenomena* (Ref. 49), Sec. 9.2.

[59] J. R. Meyer and F. J. Bartoli, J. Phys. C **15**, 1987; Phys. Rev. B **30**, 1026 (1984); **31**, 2353 (1985).

[60] J. Hubbard, Proc. R. Soc. London, Ser. A **243**, 336 (1957).

[61] L. E. Ballentine, Phys. Rev. **158**, 670 (1967); L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971); C. A. Kukkonen and A. W. Overhauser, Phys. Rev. B **20**, 550 (1979).

[62] There is reason to believe that, because the electron-electron interaction goes as $\phi_{\rm ext}\Lambda^2/\epsilon$, it should give rise anomalous transport properties when the electronic compressibility diverges. See Ref. 17.

[63] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Ref. 7), p. 142.

[64] P. Vashishta and K. S. Singwi, Phys. Rev. B **6**, 875 (1972).

[65] P. L. Reimann and A. K. Walton, Phys. Status Solidi B **48**, 161 (1971).

[66] J. Serre and A. Ghazali, Phys. Rev. B **8**, 4704 (1983).

[67] J. R. Lowney, J. Appl. Phys. **64**, 4544 (1988).