Quantum-Transport Theories and Multiple Scattering in Doped Semiconductors. II. Mobility of *n*-type Gallium Arsenide*†

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The quantum-conductivity formula derived in the previous paper is evaluated for screened Coulomb potentials. The mobility is obtained in the form $\mu=\mu_0[1+\delta_B+\delta_M+\delta_D]^{-1}$, where μ_0 is the Brooks-Herring mobility, δ_B is a correction due to higher Born approximations for the incoherent scattering, and δ_M and δ_D are, respectively, multiple scattering and dressing corrections. Analytic formulas, suitable for applications to specific semiconductors, are derived for the corrections. Applications are made to *n*-type GaAs, and it is found that the corrections are significant at all temperatures and concentrations of practical interest.

I. INTRODUCTION

IN the previous paper of this series[1] (hereafter called I) the quantum-transport theory for the impurity-limited mobility of doped isotropic semiconductors has been simplified and extended. A simple closed expression for the conductivity has been obtained which includes three distinct types of quantum corrections to the semiclassical Brooks-Herring result[2]: (1) processes in which electrons are scattered coherently from pairs of impurity centers, (2) higher Born approximations for the incoherent scattering, and (3) the dressing effects of the impurities on the electron wave functions and energy levels. However, the formula obtained still requires considerable further reduction, and some complicated integrals must be evaluated before numerical calculations are feasible. The aims of the present paper are to carry out this reduction, to obtain numerical estimates for the quantum effects in a typical *n*-type semiconductor (GaAs), and to compare the quantum theory with the Brooks-Herring theory and experiment.

We shall assume that the interaction between an electron and an ionized impurity center is of the screened-Coulomb form $V(r)=-e^2e^{-\alpha r}/(\epsilon r)$, with the screening length α^{-1} being evaluated in the long-wavelength dc limit of the random-phase approximation. The use of this screening length will certainly be justified here, since the condition for its validity (that the momentum transfer in a collision is small compared with the incident momentum) is identical with one of the criteria for the usefulness of the Born-type expansions on which the theory of I is based. A second reason for the use of the screened Coulomb potential is that the integrals involved in the relaxation time may then be evaluated by the Feynman parametric-integration technique.[3]

Gallium arsenide is a suitable semiconductor for the discussion of the quantum theory for the following reasons: (1) The conduction band is isotropic and differs only slightly from the parabolic shape[4] assumed in the theory of I. (2) The predominant scattering mechanisms near room temperature and below have been shown[4] to be due to polar lattice modes and ionized impurities. Ehrenreich has found that at room temperature the Brooks-Herring theory agrees well with experiment in the lower concentration regions where polar scattering is the more important, but that there is a discrepancy of approximately 40% at the higher concentrations, where ionized impurity scattering is dominant. (3) Gallium arsenide was thought to be important in practical applications, and hence considerable mobility data are available for it, particularly at liquid nitrogen and room temperatures. For purposes of comparison of the various theories and experiment, we have assumed uncompensated samples and used the parameters, quoted by Ehrenreich,[4] of a dielectric constant $\epsilon=13.5$ and an effective mass $m^*=0.072m$, with some adjustment where necessary for the nonparabolicity of the conduction band.[5]

The general outline of the paper is as follows. In Sec. II, the quantum-conductivity formula (I.18) is compared with the Brooks-Herring formula and quantum correction terms are defined. In Sec. III the higher Born correction for incoherent scattering is evaluated. The results are expressed in terms of the characteristic lengths of the problem, namely, the electron wavelength, the range of the impurity potential, the mean distance between impurities, and the effective Bohr radius of the ionized impurity. This correction is then calculated for uncompensated gallium arsenide as a function of temperature and impurity concentration. In Sec. IV the pair-scattering correction is examined,

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[1] E. J. Moore, preceding paper, Phys. Rev. **160**, 607 (1967).

[2] H. Brooks, Phys. Rev. **83**, 879 (1951); Advan. Electron. Electron Phys. **7**, 128 (1955).

[3] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951); J. M. Jauch and F. Rohrlich, *Theory of Photons and Electrons* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1955), Appendix A5.

[4] H. Ehrenreich, Phys. Rev. **120**, 1951 (1963).

[5] W. M. De Meis, Gordon McKay Laboratory, Harvard University, Technical Report No. ARPA-16, 1965, Fig. 4-2 (unpublished).

and in Sec. V the dressing correction is evaluated. In Sec. VI we compare the theoretical mobilities with the experimental results as a function of impurity concentration at liquid-nitrogen and room temperatures. Finally, in Sec. VII we briefly examine the region of validity of the present quantum theory.

II. DEFINITION OF THE QUANTUM CORRECTIONS

For ease of reading and for completeness it is convenient to collect here the results of paper I. It is shown there that the dc conductivity of a doped isotropic semiconductor due to ionized impurity scattering is given by[6]

$$\sigma=-(2e^2/3\hbar^2\Omega)\sum_{\mathbf{k}}(\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}})^2\tau(\mathbf{k})f_0'(\epsilon_{\mathbf{k}}), \tag{1}$$

where $f_0(\epsilon_{\mathbf{k}})=[\exp\beta(\epsilon_{\mathbf{k}}-\mu)+1]^{-1}$ is the Fermi distribution for impurity-dressed electrons (quasiparticles) of wave vector $\mathbf{k}$ and energy

$$\epsilon_{\mathbf{k}}=E_{\mathbf{k}}+(n/\Omega)\sum_{\mathbf{k}'}P(|V_{\mathbf{k}\mathbf{k}'}|^2/\omega_{\mathbf{k}\mathbf{k}'}), \tag{2}$$

with $E_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m^*$, $\omega_{\mathbf{k}\mathbf{k}'}=E_{\mathbf{k}}-E_{\mathbf{k}'}$, n the impurity concentration, and Ω the volume. The relaxation time $\tau(\mathbf{k})$ is defined by

$$1/\tau(\mathbf{k})=\sum_{\mathbf{k}'}[W_1(\mathbf{k},\mathbf{k}')+W_2(\mathbf{k},\mathbf{k}')+W_3(\mathbf{k},\mathbf{k}')+U(\mathbf{k},\mathbf{k}')]\times(1-\cos\theta_{\mathbf{k}\mathbf{k}'}), \tag{3}$$

where the transition probabilities per unit time are:

(1) The first Born approximation for incoherent scattering of the quasiparticles by the impurities,

$$W_1(\mathbf{k},\mathbf{k}')=(2n\pi/\hbar\Omega)|V_{\mathbf{k}\mathbf{k}'}|^2\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'})/\times\{[1-\Delta_{\mathbf{k}}'(E_{\mathbf{k}})][1-\Delta_{\mathbf{k}'}'(E_{\mathbf{k}'})]\}, \tag{4}$$

where

$$\Delta_{\mathbf{k}}'(E_{\mathbf{k}})=-\tfrac{1}{2}(n/\Omega)\sum_{\mathbf{k}'}|V_{\mathbf{k}\mathbf{k}'}|^2[1/(d_{\mathbf{k}\mathbf{k}'}^-)^2+1/(d_{\mathbf{k}\mathbf{k}'}^+)^2].$$

(2) The second and third Born approximations for incoherent scattering,

$$W_2(\mathbf{k},\mathbf{k}')=(2n\pi/\hbar\Omega^2)\delta(\omega_{\mathbf{k}\mathbf{k}'})\times\sum_{\mathbf{k}_1}[V(\mathbf{k}\mathbf{k}_1\mathbf{k}'\mathbf{k})/d_{\mathbf{k}\mathbf{k}_1}^-+V(\mathbf{k}\mathbf{k}'\mathbf{k}_1\mathbf{k})/d_{\mathbf{k}\mathbf{k}_1}^+] \tag{5}$$

and

$$W_3(\mathbf{k},\mathbf{k}')=\frac{2n\pi}{\hbar\Omega^3}\delta(\omega_{\mathbf{k}\mathbf{k}'})\sum_{\mathbf{k}_1\mathbf{k}_2}\left[\frac{V(\mathbf{k}\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}^-d_{\mathbf{k}\mathbf{k}_2}^-}+\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}_1\mathbf{k}'\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}^+d_{\mathbf{k}\mathbf{k}_2}^+}+\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}'\mathbf{k}_1\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}^-d_{\mathbf{k}\mathbf{k}_2}^+}\right], \tag{6}$$

where

$$V(\mathbf{k}\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_n)=V_{\mathbf{k}\mathbf{k}_1}V_{\mathbf{k}_1\mathbf{k}_2}\cdots V_{\mathbf{k}_{n-1}\mathbf{k}_n}$$

and

$$d_{\mathbf{k}\mathbf{k}_1}^{\mp}=\omega_{\mathbf{k}\mathbf{k}_1}\mp is.$$

(3) The lowest approximation for coherent scattering of the electrons from pairs of impurities,

$$U(\mathbf{k},\mathbf{k}')=\frac{2\pi n^2}{\hbar\Omega^2}\delta(\omega_{\mathbf{k}\mathbf{k}'})\sum_{\mathbf{k}_1\mathbf{k}_2}\left\{\delta_{\mathbf{k}-\mathbf{k}'+\mathbf{k}_1-\mathbf{k}_2}\left[\frac{V(\mathbf{k}\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}^-d_{\mathbf{k}\mathbf{k}_2}^-}+\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}_1\mathbf{k}'\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}^+d_{\mathbf{k}\mathbf{k}_2}^+}\right]+\delta_{\mathbf{k}+\mathbf{k}'-\mathbf{k}_1-\mathbf{k}_2}\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}'\mathbf{k}_1\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}^-d_{\mathbf{k}\mathbf{k}_2}^+}\right\}. \tag{7}$$

The semiclassical Brooks-Herring formula for the conductivity is formally identical with the quantum result (1), but with $\epsilon_{\mathbf{k}}$ replaced by the conduction-band electron energy $E_{\mathbf{k}}$, and with the relaxation time $\tau(\mathbf{k})$ replaced by the Brooks-Herring relaxation time:

$$1/\tau_0(\mathbf{k})=(2n\pi/\hbar\Omega)\sum_{\mathbf{k}'}|V_{\mathbf{k}\mathbf{k}'}|^2\delta(\omega_{\mathbf{k}\mathbf{k}'})(1-\cos\theta_{\mathbf{k}\mathbf{k}'}). \tag{8}$$

The quantum result (1) has been derived by a perturbation-expansion method which can only be expected to be valid if the differences between the quantum and the semiclassical results are relatively small. In this case it is useful to rewrite (1) in the form

$$\sigma=-\frac{2e^2}{3\hbar^2\Omega}\sum_{\mathbf{k}}\frac{(\nabla_{\mathbf{k}}E_{\mathbf{k}})^2f_0'(E_k)\tau_0(\mathbf{k})}{1+\delta_B(\mathbf{k})+\delta_M(\mathbf{k})+\delta_D(\mathbf{k})}+O(V), \tag{9}$$

where δ_B includes the effects of W_2 and W_3 and is called the incoherent Born correction. δ_M, which arises from the coherent-scattering U term, is called the multiple-scattering or pair correction. Finally, δ_D, which includes all effects arising from the impurity dressing of the electron energy levels and wave functions, is called the dressing correction. Since we are considering an isotropic semiconductor, the δ's are functions only of the magnitude of $\mathbf{k}$, i.e., of the energy $E_{\mathbf{k}}$. After integration over the angles, (9) reduces to an energy integral with integrand $E^3f_0'(E)/\{Q_0(4k^2/\alpha^2)[1+\delta_B(k)+\delta_M(k)+\delta_D(k)]\}$, where $Q_0(y)=\ln(1+y)-y/(1+y)$ is a slowly varying function in the physically interesting region of $y\gg1$. When the δ's are less than unity, the denominator will be slowly varying compared with $E^3f_0'(E)$, and hence, in the usual manner, we may remove it from the integral, evaluating it at the peak energy E_{peak} of $E^3f_0'(E)$. The formula for the quantum conductivity then reduces to the very simple and useful form

$$\sigma=\sigma_0/[1+\delta_B(k_{\text{peak}})+\delta_M(k_{\text{peak}})+\delta_D(k_{\text{peak}})], \tag{10}$$

where σ_0 is the semiclassical Brooks-Herring conductivity. We shall discuss the incoherent Born correction first, since it provides a framework for the discussion of the other corrections.

[6] We introduce $\hbar$ explicitly and set the impurity-potential parameter $\lambda=1$.

III. THE INCOHERENT BORN CORRECTION

In lowest order in the impurity potential, the Born correction is given by

$$\delta_B(k)=\tau_0(\mathbf{k})\sum_{\mathbf{k}'} W_1(\mathbf{k},\mathbf{k}')(1-\cos\theta_{\mathbf{k}\mathbf{k}'}), \tag{11}$$

where, for the screened-Coulomb-potential matrix elements $V_{\mathbf{k}\mathbf{k}'}=-(4\pi e^2/\epsilon)(|\mathbf{k}-\mathbf{k}'|^2+\alpha^2)^{-1}$, the second Born transition rate W_2 reduces to

$$W_2(\mathbf{k},\mathbf{k}')=\frac{256\pi^4e^4n}{\hbar\epsilon^2\Omega^2}\delta(\omega_{\mathbf{k}\mathbf{k}'})\,\mathrm{Re}\sum_{\mathbf{k}'}\frac{1}{d_{\mathbf{k}\mathbf{k}_1}(|\mathbf{k}-\mathbf{k}'|^2+\alpha^2)(|\mathbf{k}-\mathbf{k}_1|^2+\alpha^2)(|\mathbf{k}_1-\mathbf{k}'|^2+\alpha^2)}. \tag{12}$$

Equations (11) and (12) may be reduced to a simpler form by introducing the momentum-transfer variable $t=|\mathbf{k}-\mathbf{k}'|^2$ and using the energy δ function to carry out the $E_{\mathbf{k}'}$ integration. The result is

$$\delta_B(k)=\frac{2m^*e^2}{\pi^2\hbar^2\epsilon Q_0(4k^2/\alpha^2)}\int_0^{4k^2}\frac{t\,dt}{t+\alpha^2}F(k,t), \tag{13}$$

where

$$F(k,t)=\mathrm{Re}\int[(k_1^2-k^2+i0)(|\mathbf{k}_1-\mathbf{k}'|^2+\alpha^2)\times(|\mathbf{k}-\mathbf{k}_1|^2+\alpha^2)]^{-1}d\mathbf{k}_1. \tag{14}$$

The integration in (14) is extremely difficult to perform by direct methods, but is quite simple if the Feynman parametric-integration technique is used.[3] Using this method, several authors[3,7] have obtained the result

$$F(k,t)=\frac{2\pi^2}{[t(\alpha^4+4k^2\alpha^2+tk^2)]^{1/2}}\times\tan^{-1}\left[\frac{t\alpha^2}{4(\alpha^4+4k^2\alpha^2+tk^2)}\right]^{1/2}. \tag{15}$$

For a clearer picture of the behavior of the Born correction, it is convenient to introduce the characteristic lengths of the impurity-scattering problem. These are the electron wavelength $\lambda(=2\pi/k)$, the potential range a, which may be defined as twice the screening length, and the effective Bohr radius $a_0^*=\hbar^2\epsilon/(m^*e^2)$. These lengths are evaluated for the peak energy of $E^3f'(E)$. In terms of these lengths we obtain

$$\delta_B(k_{\mathrm{peak}})=(\lambda^2/\pi^2aa_0^*)Q_B(4\pi^2a^2/\lambda^2)=c_BQ_B(y), \tag{16}$$

where

$$Q_B(y)=\frac{y}{2Q_0(y)}\int_0^y\frac{x\,dx}{(1+x)[x(1+y+\frac{1}{4}xy)]^{1/2}}\times\tan^{-1}\left[\frac{x}{4(1+y+\frac{1}{4}xy)}\right]^{1/2} \tag{17}$$

is a function which is plotted in Fig. 1. From a knowledge of the parameters of the semiconductor, we may now evaluate readily the Born correction. For the particular case of uncompensated n-type gallium arsenide, the Born correction is plotted in Fig. 2. The qualitative behavior of these curves can be easily understood. At all temperatures and concentrations

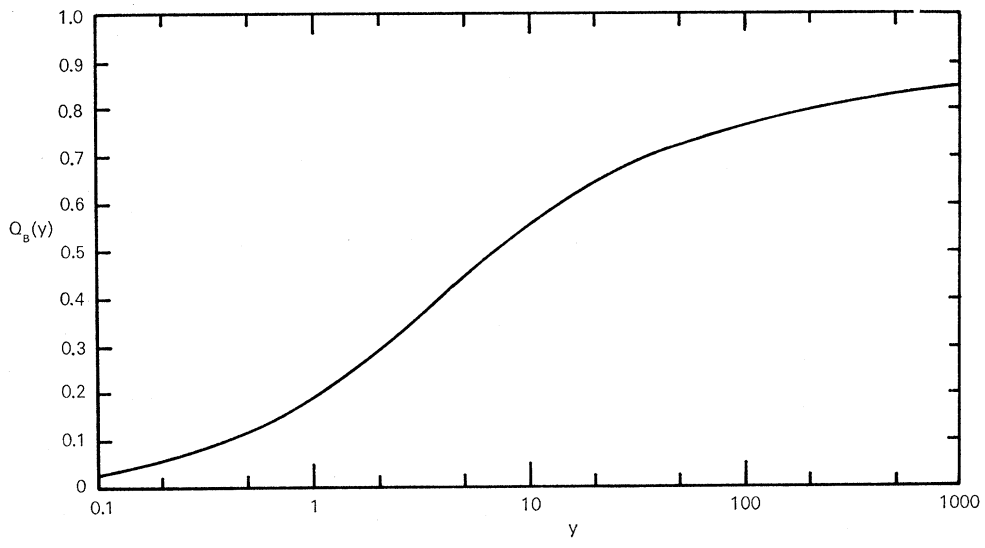

FIG. 1. The incoherent Born function $Q_B(y)$ [Eq. (17)].

[7] R. H. Dalitz, Proc. Roy. Soc. (London) **A206**, 509 (1951).

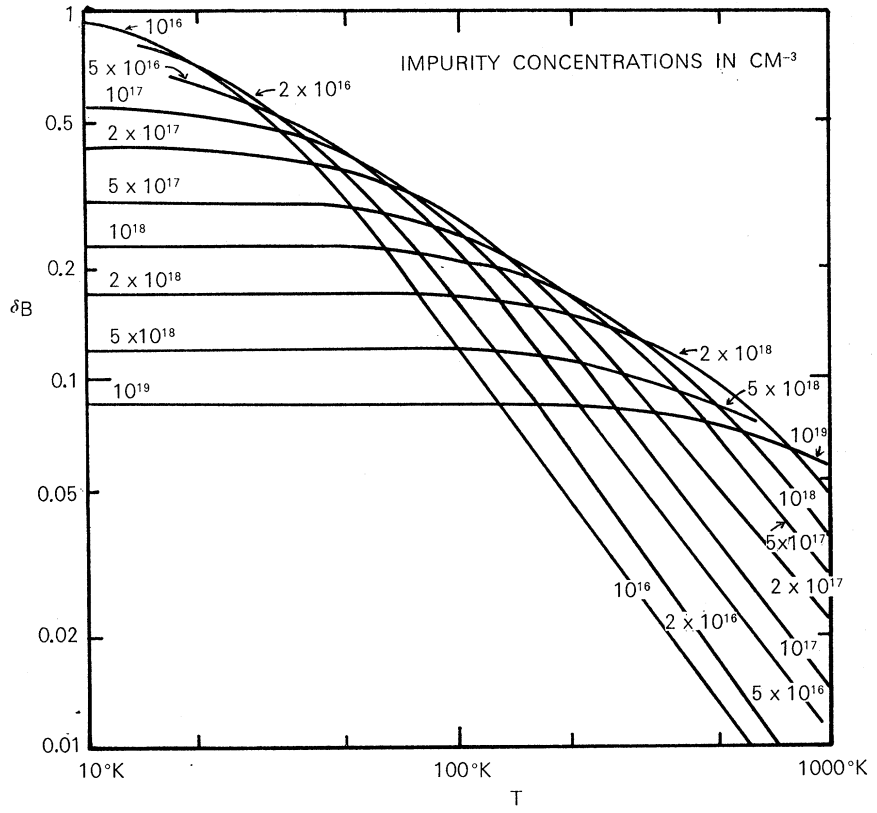

FIG. 2. Plot of the incoherent Born correction [δ_B in Eq. (10)] in uncompensated n-type GaAs versus temperature at constant impurity concentration.

shown, the parameter $y=4\pi^2a^2/\lambda^2\gtrsim 10$, and hence $Q_B(y)$ is slowly varying. The main temperature and concentration dependence of δ_B therefore comes from the parameter $c_B=\lambda^2/(\pi^2 a a_0^*)$ of (16). At the higher temperatures, the electron gas is dilute and the Boltzmann statistics apply. In this region the potential range $a\propto T^{1/2}n^{-1/2}$ and the electron wavelength $\lambda\propto T^{-1/2}$, and hence c_B behaves as $T^{-3/2}n^{1/2}$. Thus, as the temperature decreases, δ_B increases, which is consistent with the decreasing validity of the first Born approximation (cf. Blatt[8]). The decrease in temperature also results in an increasing degeneracy of the electron gas, and consequently the characteristic energy E_{peak} of the charge carriers changes from the $3\kappa T$ of the Boltzmann regime to the Fermi energy $E_F=(3\pi^2)^{2/3}\hbar^2n^{2/3}/(2m^*)$ of the degenerate regime. Hence δ_B becomes less dependent on temperature. The crossing of the curves near 100°K reflects the change in the concentration dependence of c_B from the $n^{1/2}$ characteristic of the Boltzmann regime to the $n^{-1/2}$ of the degenerate region.

Without evaluating the incoherent-scattering probability exactly it is difficult to estimate how large δ_B can be expected to become before (1) ceases to be valid. However, from previous investigations of the validity of Born expansions for Yukawa (screened-Coulomb) potentials by Jost and Pais[3] and by Dalitz,[7] it would appear that second Born corrections are useful only if they are quite small. Somewhat arbitrarily we would estimate that the Born correction is accurate for $\delta_B=10\%$, but that it is probably questionable at 30%. If we use the fact that the range of the potential is of the same order of magnitude as the effective Bohr radius, then $c_B=4/y$, and hence the condition that $\delta_B<0.3$ leads to the requirement that $y>10$.

IV. THE MULTIPLE-SCATTERING CORRECTION

The multiple-scattering correction, which may be obtained by comparing (9) with (1), is given by

$$\delta_M(k)=\tau_0(\mathbf{k})\sum_{\mathbf{k}'}U(\mathbf{k},\mathbf{k}')(1-\cos\theta_{kk'}), \qquad (18)$$

where, for the screened Coulomb potential, the pair transition rate is

$$U(\mathbf{k},\mathbf{k}')=\frac{2\pi n^2}{\hbar\Omega^2}\delta(\omega_{\mathbf{k}\mathbf{k}'})\left(\frac{4\pi e^2}{\epsilon}\right)^4\left\{2\,\mathrm{Re}\sum_{\mathbf{k}_1\mathbf{k}_2}\frac{\delta_{\mathbf{k}+\mathbf{k}_1-\mathbf{k}'-\mathbf{k}_2}}{d_{\mathbf{k}\mathbf{k}_1}-d_{\mathbf{k}\mathbf{k}_2}-(|\mathbf{k}-\mathbf{k}'|^2+\alpha^2)^2(|\mathbf{k}'-\mathbf{k}_1|^2+\alpha^2)^2}\right.$$
$$\left.+\sum_{\mathbf{k}_1\mathbf{k}_2}\frac{\delta_{\mathbf{k}+\mathbf{k}'-\mathbf{k}_1-\mathbf{k}_2}}{d_{\mathbf{k}\mathbf{k}_1}-d_{\mathbf{k}\mathbf{k}_2}+(|\mathbf{k}-\mathbf{k}_1|^2+\alpha^2)^2(|\mathbf{k}'-\mathbf{k}_1|^2+\alpha^2)^2}\right\}. \qquad (19)$$

[8] F. J. Blatt, J. Phys. Chem. Solids 1, 262 (1957).

These equations may be reduced by again introducing the momentum-transfer variable $t=|\mathbf{k}-\mathbf{k}'|^2$ and performing the $E_{\mathbf{k}'}$ integration. We find

$$\delta_M(k)=\frac{16m^{*2}ne^4}{\pi\epsilon^2\hbar^4Q_0(4k^2/\alpha^2)}\times\left\{\int_0^{4k^2}\frac{tdt}{(t+\alpha^2)^2}K(k,t)+\tfrac{1}{2}\int_0^{4k^2}tL(k,t)dt\right\},\quad(20)$$

where

$$K(k,t)=(\hbar^2/2m^*)^2\,\mathrm{Re}\int[d_{\mathbf{k}\mathbf{k}_1}{}^{-}d_{\mathbf{k},\mathbf{k}+\mathbf{k}_1-\mathbf{k}'}\times(|\mathbf{k}'-\mathbf{k}_1|^2+\alpha^2)^2]^{-1}d\mathbf{k}_1\quad(21)$$

and

$$L(k,t)=(\hbar^2/2m^*)^2\int[d_{\mathbf{k}\mathbf{k}_1}{}^{-}d_{\mathbf{k},\mathbf{k}+\mathbf{k}'-\mathbf{k}_1}{}^{+}\times(|\mathbf{k}-\mathbf{k}_1|^2+\alpha^2)^2(|\mathbf{k}'-\mathbf{k}_1|^2+\alpha^2)^2]^{-1}d\mathbf{k}_1.\quad(22)$$

The integrals in (21) and (22) are again of the type for which the Feynman parametric-integration technique was developed. The evaluation of (21) is comparatively simple, but (22) involves a long and tedius calculation. If we denote $t\alpha^{-2}$ by x and the unit step function by $\theta(u)$, the values of the integrals can be shown to be[9]

$$K(k,t)=\frac{\pi^2}{\alpha^5}\left\{\frac{1}{(1+y)(1+y-x)}+\frac{2+y-x}{x^{1/2}(1+y-x)^{3/2}}\tan^{-1}\left(\frac{x}{1+y-x}\right)^{1/2}\right\}\quad(23)$$

and

$$L(k,t)=L_1(k,t)+L_2(k,t)+L_3(k,t),\quad(24)$$

where

$$L_1(k,t)=\pi^2\alpha^{-9}\{(7/256)x^4y^2+\tfrac{1}{32}x^4y+(19/128)x^3y^2+\tfrac{1}{8}x^3y-\tfrac{1}{16}x^3+\tfrac{1}{8}x^2y^2-\tfrac{3}{8}x^2y-\tfrac{5}{8}x^2-\tfrac{1}{16}xy^2-(17/16)xy-(9/8)x+\tfrac{1}{4}y^2+\tfrac{1}{4}y\}/\{x(1+x)(1+y)\times(1+\tfrac{1}{2}x)(1+y+\tfrac{1}{4}xy)^2(1+\tfrac{1}{4}x)^2\},\quad(25)$$

$$L_2(k,t)=\frac{\pi^2(2+2x+\frac{1}{4}x^2)}{2\alpha^9(y-x)^{1/2}(1+x)^{3/2}(1+\frac{1}{2}x)^3}\times\left\{-\pi\theta\left(2\left[\frac{1+x}{x(y-x)}\right]^{1/2}-1\right)+2\tan^{-1}\left(\frac{1+x}{y-x}\right)^{1/2}\right\},\quad(26)$$

and

$$L_3(k,t)=-\pi^2(-\tfrac{1}{8}x^4y+\tfrac{1}{2}x^3y^2+\tfrac{1}{4}x^3+3x^2y^2+(15/4)x^2y+2x^2+5xy^2+9xy+5x+y^2+y)\times\tan^{-1}[x/4(1+y+\tfrac{1}{4}xy)]^{1/2}/\times[2\alpha^9x^{3/2}(1+\tfrac{1}{2}x)^3(1+y+\tfrac{1}{4}xy)^{5/2}].\quad(27)$$

The results for the multiple-scattering correction may be most conveniently presented by introducing the function

$$Q_M(y)=\frac{\alpha^5y}{2\pi^2Q_0(y)}\int_0^y\left\{\frac{x}{(1+x)^2}K(k,t)+\tfrac{1}{2}\alpha^4xL(k,t)\right\}dx.\quad(28)$$

This function, which can be evaluated easily by numerical integration on a computer, is slowly varying for $y>10$ and approaches unity for large y. $Q_M(y)$ is plotted in Fig. 3. It is unclear what physical significance, if any, should be attached to the behavior of Q_M and, in particular, to the cusp at $y=8.2$. Although one might expect resonance-type scattering to be observed under certain conditions of electron wavelength, range of potential, distance between impurities, and phase shift, the cusp occurs in a region ($y<10$), where Born expansions are either beginning to break down or are invalid.

In terms of Q_M and the characteristic lengths of the problem, namely, the range a, the electron wavelength λ, the effective Bohr radius $a_0{}^*$, and the mean distance between impurities $D=n^{-1/3}$, the multiple-scattering correction (20) can be written

$$\delta_M(k_{\mathrm{peak}})=c_MQ_M(y),\quad(29)$$

where

$$c_M=\lambda^2a^3/(4\pi a_0{}^{*2}D^3)\quad(30)$$

is called the multiple-scattering parameter. For $y>10$, Q_M is slowly varying and ranges in value between 1.6–1. The parameter c_M then provides estimates for the importance of multiple scattering. The smallness of this parameter for small λ and a bears out the physically expected result that multiple scattering should be unimportant if either the electron wavelength or the range of the potential is small compared with the mean distance between impurities. In applying (29) one must bear in mind that it has been derived by a perturbation-expansion method which assumes that the impurity potential is weak and that triplet and higher-order scattering processes can be neglected. The formula is therefore not applicable when the multiple-scattering processes are most important, as, for example, when the electron wavelength is of the same order or greater than the distance between impurities.

From Eqs. (29) and (30) and Fig. 3 one can easily evaluate the multiple-scattering correction for specific semiconductors. The results for uncompensated n-type gallium arsenide are plotted in Fig. 4 as a function of

[9] E. J. Moore, thesis, Harvard University, 1966 (unpublished); Division of Engineering and Applied Physics, Harvard University, Technical Report No. ARPA-24, 1966 (unpublished).

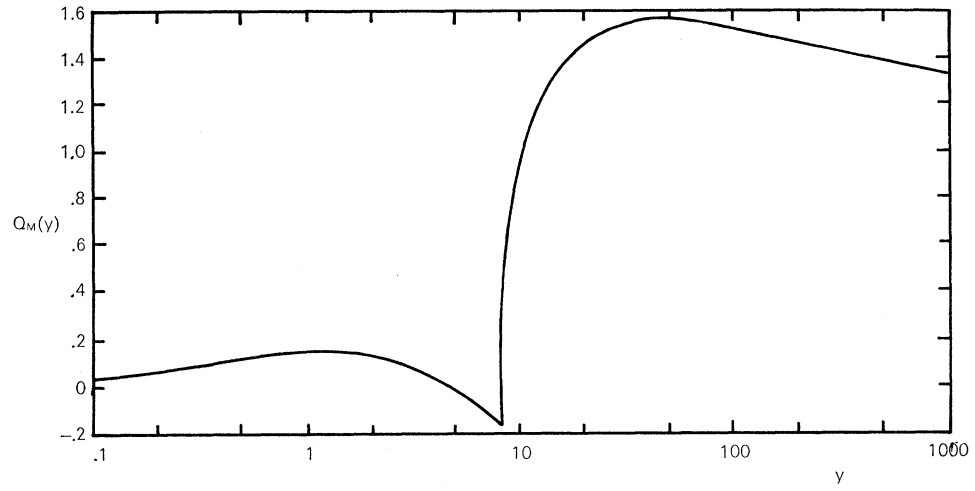

FIG. 3. The multiple-scattering function $Q_M(y)$ [Eq. (28)].

temperature for impurity concentrations between 10^{16} and 10^{19} cm^{-3}. The behavior of the curves is readily understood. For temperatures above approximately 100°K the Born parameter y is sufficiently large at all concentrations shown that the main temperature and concentration dependence of δ_M is due to the variation of c_M. At the higher temperatures the Boltzmann statistics apply, and $a \propto T^{1/2}n^{-1/2}$ and $\lambda \propto T^{-1/2}$. The temperature dependence of the range thus dominates c_M, with the variation in the electron wavelength reducing this dependence from $T^{3/2}$ to $T^{1/2}$. The result that multiple scattering becomes less important at the higher impurity concentrations may appear surprising. The explanation is that we are considering an uncompensated extrinsic semiconductor in which all the conduction electrons arise from the ionization of the impurities, and for which the electron concentration equals the impurity concentration. As the concentration increases, the electrons screen the ions more effectively, thus reducing the range of the potential. This reduction of the range dominates the concentration dependence of δ_M, although the decrease in the impurity separation D reduces this dependence from $n^{-3/2}$ to $n^{-1/2}$. At the lower temperatures the electron gas becomes more degenerate, and hence c_M is less dependent on temperature. However, at temperatures near 100°K for impurity concentrations between 5×10^{16} and 10^{18} cm^{-3}, the parameter y approaches 10 and the cusp in Q_M then leads to a marked decrease in δ_M in this region. As previously noted, the formula for δ_M is of doubtful validity in this cusp region. The minima in the 10^{18}–10^{19} cm^{-3} curves near 1000°K is due to the fact that the parameter y passes through a minimum value in the region of intermediate degeneracy. The variation of δ_M with impurity concentration is relatively insensitive to the degree of degeneracy of the electrons, with $\delta_M \propto n^{-1/2}$ in the non-

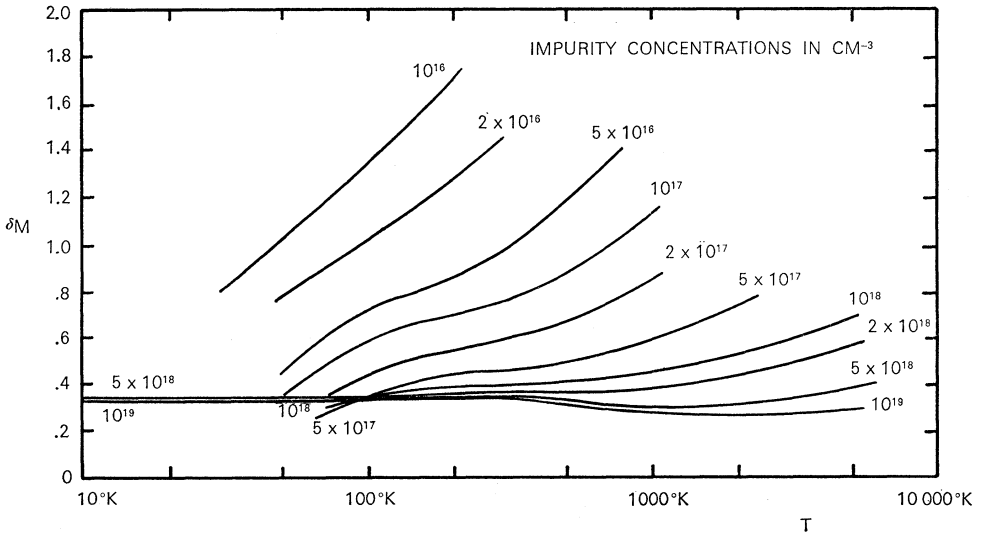

FIG. 4. Plot of the multiple-scattering correction [δ_M in Eq. (10)] in uncompensated n-type GaAs versus temperature at constant impurity concentration.

degenerate and $\delta_M \propto n^{-1/6}$ in the degenerate limit. The values of the multiple-scattering corrections are surprisingly high, and for concentrations below about 10^{18} cm^{-3} are so large that the validity of the present theory is questionable.

V. THE DRESSING CORRECTION

The dressing corrections δ_D are due to the perturbing effects of the impurities on the electronic energy levels and wave functions. Characteristic of this type of correction is the appearance of the dressing function $\Delta_{\mathbf{k}}(\omega)$. The change in the energy levels produces changes in the equilibrium distribution function $f_0(\epsilon_{\mathbf{k}})$, in the first-Born-approximation transition probability W_1, in the screening length, and in the velocity term $\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$. We shall not investigate these effects here, since it can be proved[9] that the characteristic parameter describing them is small compared with the multiple-scattering parameter in the region in which the Born expansion is useful. However, the correction due to the impurity dressing of the electron wave functions is not small and must be included. It is a relatively straightforward calculation to show that the wave-function normalization correction is given by

$$\delta_D(k)=\tau_0(\mathbf{k})\sum_{\mathbf{k}'} W_1(\mathbf{k},\mathbf{k}')(1-\cos\theta_{\mathbf{k}\mathbf{k}'})-1$$

$$=[1-\tfrac{1}{4}c_M y/(1+y)]^{-2}-1+O(c_M/y). \quad (31)$$

By comparing (31) with (29) we can see that both the multiple-scattering and the dressing correction have the same expansion parameter c_M and that, in the region in which $y>10$, δ_D is approximately 30–50% of δ_M. Although possible, it is doubtful that there is direct physical significance in the fact that c_M appears as the parameter in both the multiple-scattering and the dressing corrections, since the structure of the two terms is very different [cf. Eqs. (4) and (7)].

VI. MOBILITY OF GALLIUM ARSENIDE

The simplest method of evaluating the quantum mobility consists in first calculating the Brooks-Herring mobility and then using (10), where the values of the corrections can be obtained from Figs. 2 and 4 or from the Eqs. (16), (29), and (31). To obtain the measured mobility it is then necessary to combine the impurity mobility with the polar mobility. At 77°K the results of Ehrenreich[4] give a polar mobility in excess of 10^5 cm^2/V sec, while at room temperature the value is 9300 cm^2/V sec. In the calculations of Ehrenreich, the polar and impurity mobilities at room temperature were combined by means of a variational principle. Since this is a lengthy calculation and we expect our results to be valid only in the degenerate limit,[10] we have combined the mobilities by the formula

$$1/\mu=1/\mu_P+1/\mu_I, \quad (32)$$

which is exact when all the carriers have the same energy, as they would at the Fermi energy in the extreme degenerate case.

The results obtained for the mobilities at 77°K are shown in Fig. 5, and for those at 300°K in Fig. 6. Since polar scattering is insignificant at 77°K, the curves of Fig. 5 represent the most meaningful test of the quantum theory. In Fig. 5 the quantum mobility is compared with the Brooks-Herring mobility and with the experimental results of Woods[11] and Willardson.[12] The experimental data quoted are the highest values for a given concentration, since these presumably correspond to the least compensated samples (the actual scatter of the experimental data of Woods[11] was in fact reasonably large). The agreement between theory and experiment is surprisingly good, with the quantum curve corresponding to a parabolic band giving the best fit at all concentrations. Above 10^{18} cm^{-3}, the agreement should be quantitatively meaningful, since the corrections are sufficiently small for the theory to be valid. At lower concentrations the agreement must be regarded as somewhat fortuitous, since the Born expansion is of doubtful validity, the multiple-scattering correction is very large, and the neglect of electron-electron scattering is not justified. However, the results indicate that the inclusion of the quantum corrections produces a significant improvement between theory and experiment at all concentrations.

In Fig. 6 the theoretical curves represent: (1) the present quantum theory, with the polar and impurity mobilities combined according to (32); (2) the semiclassical theory, with the Brooks-Herring mobility and the polar mobility combined according to (32); and (3) the semiclassical variational calculation of Ehrenreich.[4] The experimental data[12,13] represent a selection of mobility values corresponding to the highest values for a given impurity concentration. The figure shows that the inclusion of the quantum corrections results in improved agreement between theory and experiment in the degenerate region between 10^{18} and 10^{19} cm^{-3}. The curve, however, does fall considerably below the values due to Willardson.[12] At lower concentrations the agreement also appears quite good, but must be regarded as fortuitous, for the same reasons as at 77°K. In addition there are two further complications. First, Eq. (32) is significantly in error, as can be seen by comparing the semiclassical curve obtained from (32)

[10] When the electrons are not degenerate, δ_M is sufficiently large that formula (1) is of questionable validity (cf. Fig. 4).

[11] J. F. Woods (private communication).

[12] R. K. Willardson (private communication).

[13] S. E. Blum (private communication); L. R. Weisberg, J. R. Woolston, and M. Glicksman, J. Appl. Phys. **29**, 1514 (1958); F. J. Reid and R. K. Willardson, J. Electron. Control **5**, 54 (1958); N. G. Ainslie, S. E. Blum, and J. F. Woods, J. Appl. Phys. **33**, 2391 (1962); J. Black and P. Lublin, *ibid.* **35**, 2462 (1964).

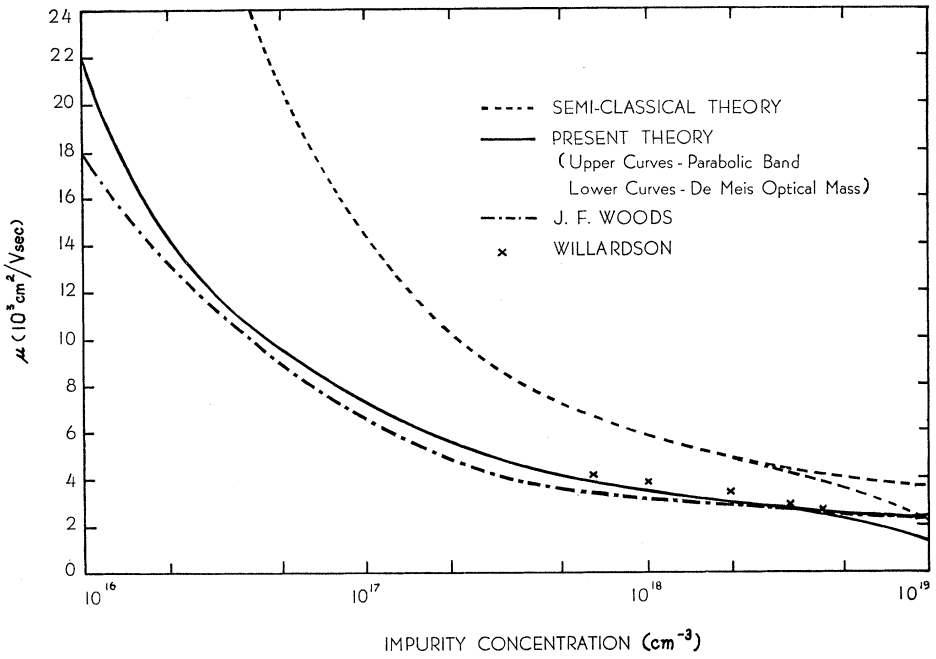

FIG. 5. Electron mobility of n-type GaAs versus impurity concentration at 77°K according to present quantum theory, Brooks-Herring theory, and experiment.

with the more exact variational curve. Second, since the pair scattering is a coherent effect, the question arises as to the validity of using the formula for δ_M when there is a second important scattering mechanism present.

VII. DISCUSSION

We have seen that for concentrations above approximately 10^{18} cm^{-3} the quantum corrections are sufficiently small that the quantum-mobility formula is valid. At these high concentrations the largest correc-

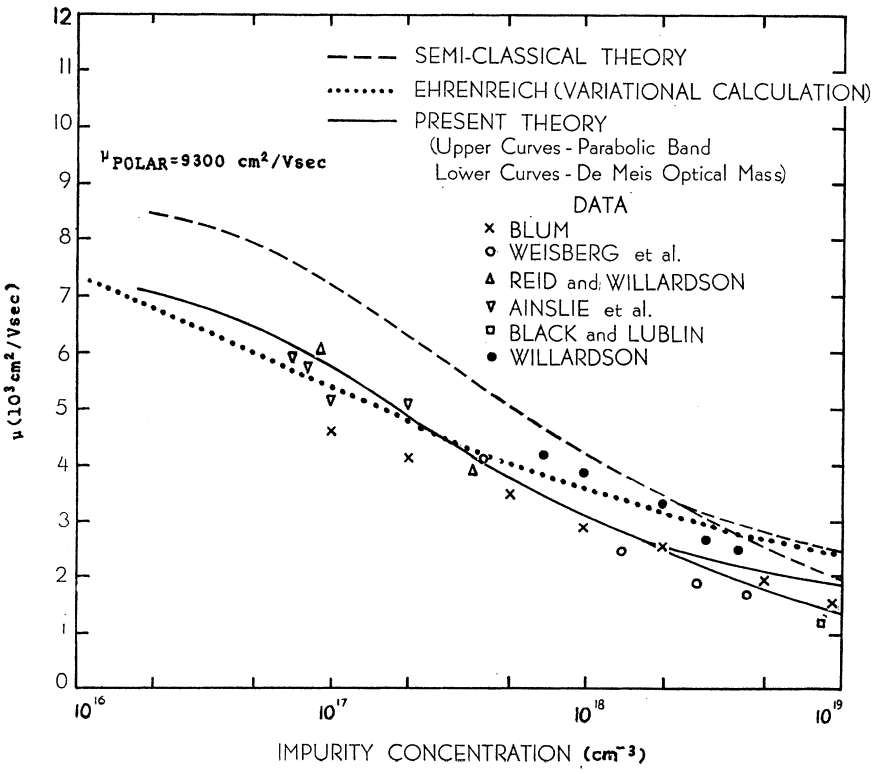

FIG. 6. Electron mobility of n-type GaAs versus impurity concentration at 300°K according to present quantum theory, semiclassical Brooks-Herring theory ($1/\mu=1/\mu_I+1/\mu_P$), Ehrenreich's variational calculation, and experiment.

tion is the multiple-scattering term, which is typically 0.35. The dressing correction and the incoherent Born correction are smaller, being in the range 0.1–0.2. We have also seen that the inclusion of these terms results in good agreement between theory and experiment. The theory of mobility in gallium arsenide in the degenerate region therefore appears fairly satisfactory.

At lower impurity concentrations, and for uncompensated samples, the theory is invalid, since the corrections become sufficiently large that the perturbation approach used in the present series of papers breaks down. This breakdown may be due to one of three reasons:

(1) The incoherent Born correction may become so large that the Born expansions are unreliable. In principle, the development of a theory which does not use Born expansions is straightforward and can be achieved by the introduction of a T matrix to describe the interaction between a quasiparticle and an impurity. This approach yields expansions in the impurity concentration, in contrast to the impurity potential expansions used here. Of the quantum theories discussed in paper I, Rickayzen[14] and Langer[15] have both used T matrices, but their theories have been restricted to lowest order in the impurity concentration. Luttinger and Kohn[16] have introduced the T matrix in a transport-equation approach and have included the coherent-scattering processes. Although numerical calculations have been carried through for the incoherent processes (Blatt[8]), no estimate of the pair terms has been made. As pointed out in Sec. I, the condition for the validity of the first Born approximation and for the applicability of the long wavelength screening is the same, and hence a T-matrix calculation should include the quantum screening effects.

(2) The multiple-scattering correction δ_M may become so large that triplet and higher-order coherent-scattering processes cannot be neglected. The theory for this general case is related to the problem of calculating the conductivity of an amorphous solid. Some progress has been made for these amorphous materials.[17]

(3) The neglect of electron-electron scattering may not be justified. In this case it will presumbaly be necessary to consider the complete many particle system as in Langer[15] and Ambegaokar.[18]

ACKNOWLEDGMENTS

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