

tering with an equilibrium phonon distribution to prove  $f_0$  Maxwellian. This is a natural consequence of the fact that elastic scattering alone cannot affect the isotropic part of the distribution.

<sup>31</sup>E. M. Conwell, *High Field Transport in Semiconductors* (Academic, New York, 1967).

<sup>32</sup>R. E. Peierls, *Quantum Theory of Solids* (Oxford U. P., London, 1964).

<sup>33</sup>G. Arlt and P. Quadflieg, *Phys. Status Solidi* **25**, 323 (1968).

<sup>34</sup>J. C. Phillips and J. A. Van Vechten, *Phys. Rev. Letters* **23**, 1115 (1969).

<sup>35</sup>C. Hilsum and A. C. Rose-Innes, *Semiconducting III-V Compounds* (Pergamon, New York, 1961).

<sup>36</sup>O. Madelung, *Physics of III-V Compounds* (Wiley, New York, 1964).

<sup>37</sup>*Semiconductors and Semimetals*, edited by R. K. Willardson and A. C. Beer (Academic, New York, 1966).

<sup>38</sup>J. M. Chamberlain and R. A. Stradling, *Solid State Commun.* **7**, 1275 (1969).

<sup>39</sup>M. Hass, in *Semiconductors and Semimetals*, edited

by R. K. Willardson and A. C. Beer (Academic, New York, 1967), Vol. III.

<sup>40</sup>K. G. Hambleton, C. Hilsum, and B. R. Holeman, *Proc. Phys. Soc. (London)* **77**, 1147 (1961).

<sup>41</sup>T. Lu, G. H. Glover, and K. S. Champlin, *Appl. Phys. Letters* **13**, 404 (1968).

<sup>42</sup>C. J. Johnson, G. H. Sherman, and R. Weil, *Appl. Opt.* **8**, 1667 (1969).

<sup>43</sup>R. K. Chang, J. M. Ralston, and D. E. Keating, in *Proceedings of the International Conference on Light Scattering Spectra of Solids* (Springer, New York, 1969).

<sup>44</sup>D. M. Chang (private communication from J. Barrera).

<sup>45</sup>H. G. B. Hicks and D. F. Manley, *Solid State Commun.* **7**, 1463 (1969).

<sup>46</sup>D. T. F. Marple, *J. Appl. Phys.* **35**, 1241 (1964).

<sup>47</sup>S. Baron and D. L. Rode (unpublished) have measured  $(1/\epsilon_\infty) \partial\epsilon_\infty/\partial T = 1.3 \times 10^{-4}/^\circ\text{K}$  for a photon energy of 0.37 eV which nearly equals the  $(1/\epsilon_0) \partial\epsilon_0/\partial T = 1.0 \times 10^{-4}/^\circ\text{K}$  reported in Ref. 41.

<sup>48</sup>J. D. Zook, *Phys. Rev.* **136**, A869 (1964).

## Properties of Electrons in Semiconductor Inversion Layers with Many Occupied Electric Subbands. I. Screening and Impurity Scattering

Eric D. Siggia\* and P. C. Kwok

*IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598*

(Received 23 December 1969)

Recently, experiments on the properties of electrons in semiconductor inversion layers have been carried out at very high electric fields. These fields correspond to electronic occupation of more than one of the discrete electric subbands created for motion perpendicular to the surface. Previous theoretical investigation on the problem was limited to the case when one subband is populated. In this paper we examine the more general case of having many subbands occupied, studying in detail two particular properties of the system. The first is the electron screening of an external potential described very conveniently by a matrix dielectric function. The second is the scattering of electrons by screened charged impurities and its contribution to the surface conductivity.

### I. INTRODUCTION

When a sufficiently strong electric field is applied across the interface of an insulator and a  $p$ -type semiconductor, an  $n$ -type inversion layer is formed in the semiconductor localized near the surface. This occurs when the conduction-band edge is bent near or below the Fermi level in the bulk. The shape of the bending is determined by the self-consistent electrostatic potential arising mainly from the electrons in the inversion layer. The self-consistent potential produces discrete levels for motion in the direction perpendicular to

the surface. These levels are known as electric subbands. The motions of the electrons in the direction parallel to the surface remain essentially Bloch-like. As the field increases, the energies of the discrete levels are lowered and at the same time their separations become larger. Eventually these subbands drop below the bulk Fermi surface in succession. In this paper we shall be concerned entirely with the properties of the inversion layers at high enough field such that several of the discrete subbands are occupied and the population in the continuum levels is negligible.<sup>1</sup>

Stern and Howard<sup>2</sup> represented the first system-

atic quantum-mechanical investigation of various properties of the electrons in the inversion layer. They calculated the electric subband wave functions in the effective-mass approximation for arbitrary orientation of the constant-energy surfaces of the conduction band. They also studied the effects of charged impurities on the inversion-layer electrons. These effects can be conveniently classified in the following ways. First of all, the charged centers will induce screening electron clouds around them. Secondly, these screened impurities give rise to scattering of the electrons and represent an important contribution to limiting the surface mobility. Finally, at low enough temperature the individual charged centers can trap electrons into bound states so that their motions in the parallel directions (on the surface) are also quantized. In contrast to the situation in three dimensions, the condition for the existence of such surface bound states is much less stringent.<sup>3</sup> However, the work of Stern and Howard is restricted to the case of only one (the lowest) electric subband being occupied. Thus their surface dielectric function is essentially one intraband element of a matrix dielectric function required in the general case when more than one subband is included in the calculation. In calculating the surface mobility due to impurity scattering, only intraband transitions are included. Furthermore, the scattering amplitude is calculated without considering the possibility of interference and multiple scattering effects, which can be appreciable because of the rather high concentration of impurities usually encountered. Recently, experimental data on the various properties of inversion layers at higher field or equivalently higher concentration of electrons in the inversion layer have become available.<sup>4</sup> They correspond to the situation in which more than one subband is occupied. Therefore, in order to understand these new results from a theoretical viewpoint one must extend the work of Stern and Howard to include multiband effects. It is in this spirit of providing a broader theoretical basis for future comparison with experiments that the present paper is prepared.

In Sec. II A, a review of the calculation of the electric subbands in the effective-mass approximation is presented. Screening of charged impurities by electrons occupying discrete electric subbands is considered in Sec. II B. A matrix dielectric function is calculated both in the Hartree approximation and in the random-phase approximation (RPA). In Sec. II C, the dielectric function is evaluated approximately for some limiting cases. Section III is devoted to the calculation of electron surface mobility due to impurity scattering. In Sec. III A, the problem of scattering by a single

impurity of the electrons in the discrete electric subbands is formulated. Expressions for the scattering cross sections which include intersubband scattering are derived. In Sec. III B, the study is extended to the actual case of many scattering centers. Interference and multiple scattering effects which give rise to corrections to the simple result that the total cross section is equal to the sum of the individual ones are examined. In Sec. III C, the surface conductivity is derived by solving approximately a set of coupled Boltzmann's equations describing the distribution functions of the electrons in different electric subbands. Finally a few concluding remarks are made in Sec. IV.

## II. SURFACE DIELECTRIC FUNCTION

### A. Review of Electric Subband Calculation

We begin by summarizing the calculation of electric subbands in the effective-mass approximation. This will also serve to define the various quantities referred to later. The wave function of an electron in the inversion layer belonging to a particular valley  $v$  is described by the product function  $e^{i\vec{k}_v \cdot \vec{r}} \times u_v(\vec{r})\psi^v(\vec{r})$ , where  $\vec{k}_v$  is the wave vector and  $u_v(\vec{r})$  is the periodic part of the Bloch function at the bottom of the valley. The envelope function  $\psi^v(\vec{r})$  satisfies the Schrödinger equation

$$(T^v + V - E)\psi^v = 0 .$$

The derivation of such an equation may be found in the review article by Kohn.<sup>5</sup> It depends on the assumption that interband and intervalley matrix elements of the external potential are small and can be neglected. This is a valid assumption if  $V$  varies negligibly over a distance of the order of the size of a unit cell. In the present case, the above criterion is not quite satisfied because our potential, taken simply to be infinite in the insulator ( $z < 0$ ) and equal to the self-consistent electrostatic potential  $-e\phi(z)$  in the semiconductor ( $z > 0$ ),<sup>2</sup> is rapidly varying near the surface. It is beyond the scope of this paper to elaborate on this question, and we shall proceed with the equation

$$\begin{aligned} (T^v - e\phi(z) - E)\psi^v &= 0 , & z \geq 0 \\ \psi^v &= 0 , & z = 0 . \end{aligned} \quad (1)$$

The operator  $T^v$  is the kinetic energy operator

$$T^v = \frac{1}{2} \sum_{ij} w_{ij}^v \left( \frac{\hbar}{i} \frac{\partial}{\partial x_i} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x_j} \right) , \quad (2)$$

where  $w_{ij}^v$  is the inverse effective-mass tensor defined in our particular coordination system.  $\phi(z)$ , as mentioned above, is the electrostatic potential and is determined from the Poisson equation

$$\frac{\partial^2}{\partial z^2} \phi(z) = -\frac{4\pi}{\kappa_{sc}} [\rho(z) + \rho_d(z)] , \quad z > 0 \quad (3)$$

with the boundary condition

$$\kappa_{\text{ins}} \frac{\partial \phi}{\partial z} \Big|_{z=0^-} = \kappa_{\text{sc}} \frac{\partial \phi}{\partial z} \Big|_{z=0^+}, \quad \lim_{z \rightarrow +\infty} \phi(z) = 0. \quad (4)$$

The quantities  $\kappa_{\text{sc}}$  and  $\kappa_{\text{ins}}$  represent the dielectric constant of the host semiconductor and the insulator, respectively. The charge density in (3) consists of two parts. One part which may be considered as known is the fixed negatively charged acceptor centers in the depletion layer. This part has been approximated by the smooth function  $\rho_d(z)$ . The other part is the charge density  $\rho(z)$  of the electrons in the inversion layer, given self-consistently by<sup>6</sup>

$$\rho(z) = 2 \sum_v \sum_n |\psi_n^v(xy, z)|^2 f(E_n^v), \quad (5)$$

where  $\psi_n^v$  and  $E_n^v$  are the eigenfunctions and eigenvalues of the Schrödinger equation [Eqs. (1)] and  $f$  is the Fermi distribution function. In (5), the total electron wave function  $e^{i\vec{k}_v \cdot \vec{r}} \psi_n^v(\vec{r})$  is simply replaced by the envelope function. This approximation is reasonable because the inverse Laplace operator  $[(\nabla^2)^{-1}]$  has a smoothing-out effect. The quantity  $|\psi_n^v|^2$  will be shown to be independent of  $x$  and  $y$ .

The eigenfunctions and eigenvalues of Eq. (1) are readily found to be<sup>2</sup>

$$\begin{aligned} \psi_{\alpha \vec{k}}^v(\vec{r}) &= (1/\sqrt{A}) e^{i\vec{k} \cdot \vec{r}} e^{-i(\vec{w}^v \cdot \vec{k})z} \xi_{\alpha}^v(z), \\ E_{\alpha \vec{k}}^v &= \epsilon_{\alpha}^v + E_{\vec{k}}^v, \\ E_{\vec{k}}^v &= \frac{1}{2} \hbar^2 [(w_{11} - w_{13}^2/w_{33})^v k_x^2 \\ &\quad + (w_{12} - w_{13}w_{23}/w_{33})^v k_x k_y \\ &\quad + (w_{22} - w_{23}^2/w_{33})^v k_y^2], \end{aligned} \quad (6)$$

where the following abbreviations have been used:

$$\begin{aligned} \vec{k} &= k_x \hat{x} + k_y \hat{y}, \\ \vec{\rho} &= x \hat{x} + y \hat{y}, \\ \vec{w}^v &= (w_{13}^v/w_{33}^v) \hat{x} + (w_{23}^v/w_{33}^v) \hat{y}. \end{aligned} \quad (7)$$

$A$  is the area of the surface and will be taken to be unity from now on, and  $\xi_{\alpha}^v(z)$  is the eigenfunction with eigenvalue  $\epsilon_{\alpha}^v$  of the one-dimensional Hamiltonian

$$\left( -\frac{\hbar^2}{2m_3^v} \frac{d^2}{dz^2} - e\phi(z) \right) \xi_{\alpha}^v(z) = \epsilon_{\alpha}^v \xi_{\alpha}^v(z), \quad (8)$$

$$m_3^v = (w_{33}^v)^{-1}.$$

We see immediately that  $|\psi_n^v|^2 = |\psi_{\alpha k}^v|^2 = |\xi_{\alpha}^v(z)|^2$  is independent of  $x$  and  $y$  (or  $\vec{\rho}$ ). In fact, the charge density  $\rho(z)$  which enters into the Poisson equation for  $\phi(z)$  is simply

$$\rho(z) = 2 \sum_v \sum_{\alpha \vec{k}} |\xi_{\alpha}^v(z)|^2 f(E_{\alpha \vec{k}}^v). \quad (9)$$

The problem now reduces to the self-consistent determination of the wave functions  $\xi_{\alpha}^v$  and energies  $\epsilon_{\alpha}^v$  using Eqs. (3), (4), (8), and (9). For final comment, we calculate the total number of electrons in the inversion layer  $N_{\text{inv}}$ . Since  $N_{\text{inv}} = -(1/e) \int_0^{\infty} dz \rho(z)$ , one can immediately obtain the desired result by integrating Eq. (3) and making use of Eq. (4) as

$$\begin{aligned} N_{\text{inv}} &= -\frac{1}{4\pi e} \kappa_{\text{ins}} \frac{\partial \phi(z)}{\partial z} \Big|_{z=0^-} - N_{\text{depl}} \\ &= \frac{1}{4\pi e} \kappa_{\text{ins}} E^{(-)} - N_{\text{depl}}, \end{aligned} \quad (10)$$

where  $E^{(-)}$  is the electric field in the insulator and  $N_{\text{depl}} = -(1/e) \int_0^d \rho_d(z) dz = N_A d$ , the number of acceptor centers in the depletion layer of thickness  $d$ .<sup>7</sup>

#### B. Screening of Charged Impurities and Matrix Dielectric Function

We are now in a position to determine the effects on the electron system by the introduction of a charged impurity. In this section, we shall calculate the screening charge, using the familiar RPA. The result is expressed in terms of a matrix dielectric function relating the matrix elements between subband wave functions ( $\xi_{\alpha}^v$ ) of the total effective impurity potential to those of the bare or external impurity potential.

From linear-response theory the charge induced by an external potential  $V_{\text{ext}}(\vec{r})$  is given by<sup>8</sup>

$$\begin{aligned} \rho_{\text{ind}}(\vec{r}) &= 2e^2 \sum_v \sum_{nm} \psi_n^v(\vec{r}) \psi_m^{v*}(\vec{r}) \\ &\quad \times \{ [f(E_n^v) - f(E_m^v)] / (E_n^v - E_m^v + i\epsilon) \} \\ &\quad \times \int d^3 r' \psi_n^{v*}(\vec{r}') \psi_m^v(\vec{r}') V_{\text{ext}}(\vec{r}') \quad (z \geq 0) \\ &= 0 \quad (z < 0), \end{aligned} \quad (11)$$

where the total wave functions are again replaced by the envelope functions and the terms corresponding to the intervalley contributions are omitted. The latter parts are proportional to factors like  $\exp[i(\vec{k}_v - \vec{k}_{v'}) \cdot \vec{r}]$ . This approximation is consistent with the approximation we have made so far. Substituting (6) into (11), one obtains after a simple change of variable

$$\begin{aligned} \rho_{\text{ind}}(\vec{r}) &= 2e^2 \sum_v \sum_{\alpha \alpha', \vec{q}} \xi_{\alpha}^v(z) \xi_{\alpha'}^{v*}(z) e^{-i(\vec{w}^v \cdot \vec{q})z} e^{i\vec{q} \cdot \vec{r}} \\ &\quad \times L^{\alpha \alpha'}(v, \vec{q}) V_{\text{ext}}^{\alpha \alpha'}(v, \vec{q}) \quad (z \geq 0) \\ &= 0 \quad (z < 0), \end{aligned} \quad (12)$$

$$\text{where } L^{\alpha \alpha'}(v, \vec{q}) = \sum_{\vec{k}} \frac{f(E_{\alpha \vec{k}}^v) - f(E_{\alpha' \vec{k}-\vec{q}}^v)}{E_{\alpha \vec{k}}^v - E_{\alpha' \vec{k}-\vec{q}}^v + i\epsilon} \quad (13)$$

and

$$V_{\text{ext}}^{\alpha \alpha'}(v, \vec{q}) = \int d^2 \rho' dz' \xi_{\alpha}^{v*}(z') \xi_{\alpha'}^v(z')$$

$$\times e^{i(\vec{w} \cdot \vec{q})z'} e^{-i\vec{q} \cdot \vec{p}'} V_{\text{ext}}(\vec{r}') . \quad (14)$$

The potential due to the induced charge is deter-

mined by the Poisson equation with the same boundary conditions as in Eqs. (4). Explicitly, one finds<sup>9</sup>

$$\begin{aligned} V_{\text{ind}}(\vec{p}, z) &= \frac{2}{\kappa_{\text{sp}} + \kappa_{\text{ins}}} \int_0^\infty d^2\rho' \int_0^\infty dz' \frac{\rho_{\text{ind}}(\vec{\rho}', z')}{|(\vec{p} - \vec{\rho}')^2 + (z - z')^2|^{1/2}} \quad (z < 0) \\ &= \frac{1}{\kappa_{\text{sc}}} \int_0^\infty d^2\rho' \int_0^\infty dz' \frac{\rho_{\text{ind}}(\rho', z')}{|(\vec{p} - \vec{\rho}')^2 + (z - z')^2|^{1/2}} + \frac{\kappa_{\text{sc}} - \kappa_{\text{ins}}}{\kappa_{\text{sc}}(\kappa_{\text{sc}} + \kappa_{\text{ins}})} \int_0^\infty d^2\rho' \int_0^\infty dz' \frac{\rho_{\text{ind}}(\vec{\rho}', z')}{|(\vec{p} - \vec{\rho}')^2 + (z + z')^2|^{1/2}} \quad (z > 0) . \end{aligned} \quad (15)$$

For convenience, Eq. (15) will be summarized as

$$V_{\text{ind}}(\vec{p}, z) = \int d^2\rho' \int_0^\infty dz' g(\vec{p} - \vec{\rho}'; z, z') \rho_{\text{ind}}(\vec{\rho}', z') , \quad (16)$$

where the Green's function  $g$  is defined as

$$\begin{aligned} g(\vec{p} - \vec{\rho}'; z, z') &= [2/(\kappa_{\text{sc}} + \kappa_{\text{ins}})] |(\vec{p} - \vec{\rho}')^2 + (z - z')^2|^{-1/2} \quad (z < 0) \\ &= (1/\kappa_{\text{sc}}) |(\vec{p} - \vec{\rho}')^2 + (z - z')^2|^{-1/2} \\ &\quad + (\kappa_{\text{sc}} - \kappa_{\text{ins}})/[\kappa_{\text{sc}}(\kappa_{\text{sc}} + \kappa_{\text{ins}})] \\ &\quad \times |(\vec{p} - \vec{\rho}')^2 + (z + z')^2|^{-1/2} \quad (z \geq 0) . \end{aligned} \quad (17)$$

Now we may define matrix elements of the induced potential similar to these of  $V_{\text{ext}}$  defined in Eq. (14). One then finds, making use of (12), the relation

$$V_{\text{ind}}^{\alpha\alpha'}(v, \vec{q}) = \sum_{v', \alpha\alpha'} \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) V_{\text{ext}}^{\alpha\alpha'}(v', \vec{q}) \quad (18)$$

with

$$\begin{aligned} \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) &= 2e^2 \int d^2\rho e^{-i\vec{q} \cdot \vec{\rho}} \\ &\quad \times \left[ \int_0^\infty dz \int_0^\infty dz' \zeta_{\gamma'}^{v*}(z) \zeta_{\gamma'}^v(z) e^{i(\vec{w} \cdot \vec{q})z} \right. \\ &\quad \times \zeta_{\alpha'}^{v'}(z') \zeta_{\alpha'}^{v'*}(z') e^{-i(\vec{w} \cdot \vec{q})z'} g(\vec{\rho}; z, z') \left. \right] \\ &\quad \times L^{\alpha\alpha'}(v', \vec{q}) . \end{aligned} \quad (19)$$

The total potential  $V_{\text{tot}}$  is the sum of the external and the induced potential. In the present approximation its matrix element is therefore given by

$$\begin{aligned} V_{\text{tot}}^{\alpha\alpha'}(v, \vec{q}) &= \sum_{v', \alpha\alpha'} [\delta_{vv'} \delta_{\gamma\alpha} \delta_{\gamma'\alpha'} + \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q})] \\ &\quad \times V_{\text{ext}}^{\alpha\alpha'}(v', \vec{q}) . \end{aligned} \quad (20)$$

Equation (20) defines the two-dimensional  $q$ -dependent matrix dielectric function in the Hartree approximation

$$V_{\text{tot}}^{\alpha\alpha'}(v, \vec{q}) = \sum_{v', \alpha\alpha'} (\epsilon_H^{-1})_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) V_{\text{ext}}^{\alpha\alpha'}(v', \vec{q}) , \quad (21)$$

that is,

$$(\epsilon_H^{-1})_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) = \delta_{vv'} \delta_{\gamma\alpha} \delta_{\gamma'\alpha'} + \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) . \quad (22)$$

In this approximation, the induced charge is calculated to first order in the external potential [see Eq. (11) or (12)]. A better approximation is the RPA, in which one calculates the induced charge as resulting from a linear response to the total potential instead of the external potential. In other words,  $\rho_{\text{ind}}^{\text{RPA}}$  is given by (11) or (12) with  $V_{\text{ext}}$  replaced by  $V_{\text{tot}}$ . Then one obtains, instead of (20),

$$\begin{aligned} \sum_{v', \alpha\alpha'} [\delta_{vv'} \delta_{\gamma\alpha} \delta_{\gamma'\alpha'} - \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q})] V_{\text{tot}}^{\alpha\alpha'}(v', \vec{q}) \\ = V_{\text{ext}}^{\alpha\alpha'}(v, \vec{q}) \end{aligned} \quad (23)$$

and the dielectric function in the RPA

$$(\epsilon_{\text{RPA}})^{\alpha\alpha'}_{\gamma\gamma', \alpha\alpha'}(\vec{q}) = \delta_{vv'} \delta_{\gamma\alpha} \delta_{\gamma'\alpha'} - \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) . \quad (24)$$

### C. Approximate Expressions for Dielectric Function

In this subsection we shall evaluate several approximate expressions for the matrix dielectric function. First of all, the dominant matrix elements of  $\epsilon$  or  $\chi$  in the long-wavelength or zero- $q$  limit will be calculated. Secondly, one diagonal matrix element of  $\epsilon$ , valid for all  $q$ , will be evaluated for a particularly simple choice of wave function  $\zeta(z)$ . To begin, we put the susceptibility function  $\chi$ , given by (19), into a more useful form by Fourier analyzing the Green's function  $g$  according to

$$\begin{aligned} \frac{1}{|(\vec{p} - \vec{\rho}')^2 + (z \pm z')^2|^{1/2}} &= \int \frac{d^2q}{(2\pi)^2} \int \frac{dq_z}{(2\pi)} \\ &\quad \times \exp[iq \cdot (\vec{p} - \vec{\rho}') + iq_z(z \pm z')] \frac{4\pi}{q^2 + q_z^2} . \end{aligned} \quad (25)$$

The result for  $\chi$  is

$$\begin{aligned} \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) &= \frac{4\pi e^2}{q} \left[ \int_{-\infty}^{\infty} \frac{d\xi}{\pi} \frac{1}{1+\xi^2} \right. \\ &\times \left( \frac{1}{\kappa_{sc}} M_{\gamma\gamma'}^v(\vec{q}, \xi) M_{\alpha\alpha'}^{v'*}(\vec{q}, \xi) + \frac{\kappa_{sc} - \kappa_{ins}}{\kappa_{sc}(\kappa_{sc} + \kappa_{ins})} \right. \\ &\left. \left. \times M_{\gamma\gamma'}^v(\vec{q}, \xi) M_{\alpha\alpha'}^{v'*}(\vec{q}, -\xi) \right) \right] L^{\alpha\alpha'}(v', \vec{q}), \quad (26) \end{aligned}$$

where

$$M_{\gamma\gamma'}^v(\vec{q}, \xi) = \int_0^\infty dz \xi_\gamma^{v*}(z) \xi_{\gamma'}^v(z) \exp[i(\vec{w}^v \cdot \vec{q} + \xi q)z]. \quad (27)$$

In the limit of  $q \rightarrow 0$ , one obtains from (27)

$$\lim_{q \rightarrow 0} M_{\gamma\gamma'}^v(\vec{q}, \xi) = \delta_{\gamma\gamma'}, \quad (28)$$

and from (13)

$$\lim_{q \rightarrow 0} L^{\alpha\alpha'}(v, \vec{q}) = \sum_{\vec{k}} \frac{\partial}{\partial E_{\alpha\vec{k}}^v} f(E_{\alpha\vec{k}}^v). \quad (29)$$

At zero temperature the right-hand side of (29) is simply the density of states at the Fermi level for electrons occupying the  $\alpha$  subband. It is of course zero for an unoccupied subband. Using the expression in Eqs. (6) for  $E_{\alpha\vec{k}}^v$ , we get

$$\begin{aligned} \lim_{q \rightarrow 0} L^{\alpha\alpha'}(v, \vec{q}) &= -N(v) = -(1/2\pi\hbar^2) (m_1^v m_2^v)^{1/2}, \\ m_1^v &= [(w_{11} - w_{13}^2/w_{33})^v]^{-6}, \\ m_2^v &= [(w_{22} - w_{23}^2/w_{33})^v]^{-1}. \end{aligned} \quad (30)$$

An interesting feature of the limiting value of  $L^{\alpha\alpha'}$  is that it is independent of the Fermi energy or, equivalently, of the number of electrons in the inversion layer. This is the result of the constant density of states in two dimensions. Putting (28) and (30) into (26) we obtain

$$\begin{aligned} \lim_{q \rightarrow 0} \chi_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) &= (4\pi e^2/q\bar{\kappa}) \delta_{\gamma\gamma'} \delta_{\alpha\alpha'} N(v'), \\ &\quad (v' \alpha) \text{ occupied} \quad (31) \\ &= 0, \quad \text{otherwise;} \\ \bar{\kappa} &= \frac{1}{2} (\kappa_{sc} + \kappa_{ins}). \end{aligned}$$

Therefore, from (24)

$$\begin{aligned} \lim_{q \rightarrow 0} (\epsilon_{RPA})_{\gamma\gamma', \alpha\alpha'}^{vv'}(\vec{q}) &= \delta_{vv'} \delta_{\gamma\alpha} \delta_{\gamma'\alpha'} \\ &+ (4\pi e^2/q\bar{\kappa}) \delta_{\gamma\gamma'} \delta_{\alpha\alpha'} N(v'), \\ &\quad (v' \alpha) \text{ occupied} \\ &= \delta_{vv'} \delta_{\gamma\alpha} \delta_{\gamma'\alpha'}, \quad \text{otherwise.} \end{aligned} \quad (32)$$

We calculate the screening of an external potential for this dielectric function when only the lowest subband in each of the degenerate valleys is occupied. From (23) and (32), we obtain

$$V_{\text{tot}}^{00}(v, \vec{q}) + (4\pi e^2/\bar{\kappa}q) \sum_{v'} N(v') V_{\text{tot}}^{00}(v', \vec{q}) = V_{\text{ext}}^{00}(v, \vec{q}), \quad (33)$$

where the lowest subband is denoted by 0 and the sum is over the valleys degenerate with  $v$ . If we assume that the matrix elements of the screened potential and the density of state  $N(v')$  are the same for all the valleys, the above equation can be solved to yield the simple result

$$\begin{aligned} V_{\text{tot}}^{00}(v, \vec{q}) &= [(1+s/q)]^{-1} V_{\text{ext}}^{00}(v, \vec{q}), \\ s &= 2Nv [e^2(m_1 m_2)^{1/2}/\bar{\kappa}\hbar^2], \end{aligned} \quad (34)$$

where  $n_v$  is the number of degenerate valleys. This result agrees with that obtained by Stern<sup>10</sup> and shows that screening in two dimensions in the long-wavelength limit is independent of electron concentration. The situation is different in three dimensions where screening increases with electron concentration.<sup>11</sup>

Next we evaluate a diagonal matrix element of  $\chi$  or  $\epsilon$  for an arbitrary value of  $q$ , namely,  $\epsilon_{00,00}^{vv}(q)$ . Our goal is to obtain an analytic expression that is capable of illustrating the essential feature of the exact result. This can be done by making the following simplifications. We take the energy surface of our valley  $v$  to be isotropic, characterized by an "average" mass  $M = (m_1^v m_2^v)^{1/2}$ ; and the wave function  $\xi_0(z)$  to be of the simple form<sup>12</sup>

$$\xi_0(z) = [z/(2d_0^3)^{1/2}] e^{-z/2d_0},$$

and the temperature to be zero. Then we can perform all the integrals in  $L^{00}(v, \vec{q})$  [Eq. (13)] and in  $\chi_{00,00}^{vv}(\vec{q})$  [Eq. (26)] and obtain

$$\begin{aligned} L^{00}(v, \vec{q}) &= (M/2\pi\hbar^2) 2\Theta(q)/\pi, \\ \epsilon_{00,00}^{vv}(q) &= 1 + \frac{4\pi e^2}{\bar{\kappa}q} \left( \frac{M}{2\pi\hbar^2} \frac{2\Theta(q)}{\pi} \right) \\ &\times \left\{ \frac{\kappa}{\kappa_{sc}} \left[ \frac{1}{2} \left( \frac{1}{1+d_0q} \right) - \frac{1}{4} \left( \frac{1}{1+d_0q} \right)^2 \right. \right. \\ &\left. \left. + \frac{1}{4} \left( \frac{1}{1+d_0q} \right)^3 \right] + \frac{\kappa_{sc} - \kappa_{ins}}{2\kappa_{sc}} \left( \frac{1}{1+d_0q} \right)^6 \right\}, \\ \Theta(q) &= \frac{1}{2} \pi, \quad q < 2k_F \\ &= \sin^{-1}(2k_F/q), \quad q > 2k_F. \end{aligned} \quad (35)$$

The quantity  $k_F$  is the Fermi wave number and is determined as usual by the electron number. In the simple case where only the lowest subbands of the  $n_v$  degenerate valleys are occupied (with the

same isotropic mass  $M$ ) we have

$$k_F = (2\pi N_{1nv}/n_v)^{1/2}. \quad (36)$$

### III. SURFACE MOBILITY DUE TO IMPURITY SCATTERING

#### A. Formulation of Impurity Scattering

In the previous sections the total or effective potential due to an impurity introduced into the vicinity of the inversion layer was calculated. In the following sections we study the electrons by the screened impurities and their contribution to the surface mobility. The Schrödinger equation for the envelope function in the presence of an impurity becomes

$$[H_0^v + V(r)]\psi^v(r) = E\psi^v(r), \quad (37)$$

where the  $H_0^v$  is the unperturbed Hamiltonian  $T^v - e\phi(z)$  and  $V(r) = V_{\text{tot}}(r)$ . In arriving at the effective-mass equation (37), terms describing intervalley scattering have been neglected. This approximation is valid if the screened potential is slowly varying compared to factors like  $e^{i\vec{k}_v \cdot r}$ . Following standard procedure,<sup>13</sup> we solve for the outgoing wave solution to Eq. (37), obtaining

$$\psi^{(+)}(\vec{r}) = \phi_0(\vec{r}) - \int d^3r' G^{(+)}(\vec{r}, \vec{r}') V(\vec{r}') \psi^{(+)}(\vec{r}'), \quad (38)$$

where  $\phi_0(r)$  is an incident wave function,

$$\phi_0(\vec{r}) = \zeta_{\alpha_0}(z) e^{i(\vec{w} \cdot \vec{k}_0)z} e^{i\vec{k}_0 \cdot \vec{p}}. \quad (39)$$

The valley index  $v$  has been dropped for convenience. The outgoing Green's function  $G^{(+)}$  satisfies the source equation

$$[H_0 - (E + i\epsilon)] G^{(+)}(\vec{r}, \vec{r}') = \delta'(\vec{r} - \vec{r}'). \quad (40)$$

The prime on the  $\delta$  function denotes that it is defined only in the half-space  $z, z' > 0$ . In terms of the eigenfunctions of  $H_0$  [Eqs. (6)],  $G^{(+)}(r, r')$  can be written explicitly as

$$\begin{aligned} G^{(+)}(\vec{r}, \vec{r}') &= G^{(+)}(\vec{p} - \vec{p}'; z, z') \\ &= \sum_{\alpha\vec{k}} e^{i\vec{k} \cdot (\vec{p} - \vec{p}')} \zeta_{\alpha}(z) \zeta_{\alpha}^*(z') \\ &\times \exp[i(\vec{w} \cdot \vec{k})(z - z')] \left( \frac{1}{E_{\alpha\vec{k}} - E - i\epsilon} \right), \quad (41) \end{aligned}$$

where the completeness condition for the  $\zeta$  functions,

$$\sum_{\alpha} \zeta_{\alpha}(z) \zeta_{\alpha}(z') = \delta(z - z'), \quad z, z' > 0,$$

has been used. We shall pick the coordinate sys-

tem introduced in (31), i. e.,  $w_{12}^v = w_{13}^v w_{23}^v / w_{33}^v$ , so that

$$E_{\alpha\vec{k}} = (\hbar^2/2m_1)k_x^2 + (\hbar^2/2m_2)k_y^2. \quad (42)$$

The off-diagonal elements  $w_{13}^v$  and  $w_{23}^v$  are, in general, not zero unless the  $z$  axis coincides with a principal axis of the constant-energy surface. The above transformation cannot affect the values of the surface-transport coefficients, which are calculated as a sum of independent contributions from the different valleys.

The calculation of the scattering amplitudes is carried out by first obtaining the asymptotic expression for  $G^{(+)}$ , i. e., as  $|\rho| \rightarrow \infty$  along a certain direction. The  $k$  integration is best performed by changing to the new variable  $\bar{k}$ :

$$k_x = (m_1/m_2)^{1/4} \bar{k}_x, \quad k_y = (m_2/m_1)^{1/4} \bar{k}_y, \quad (43)$$

so that

$$E_{\alpha\vec{k}} = (\hbar^2/2M)\bar{k}^2 + \epsilon_{\alpha}, \quad M = (m_1 m_2)^{1/2}. \quad (44)$$

Now, integrating over the angle, we obtain

$$\begin{aligned} G^{(+)}(\vec{r}, \vec{r}') &= \sum_{\alpha} \frac{2M}{\hbar^2} \int_0^{\infty} \frac{\bar{k} d\bar{k}}{(2\pi)} \\ &\times \frac{J_0(\bar{k}R)}{\bar{k}^2 - (2m/\hbar^2)(E - \epsilon_{\alpha}) - i\epsilon} \zeta_{\alpha}(z) \zeta_{\alpha}(z'), \quad (45) \end{aligned}$$

where  $J_0$  is the zero-order cylindrical Bessel function<sup>14</sup> and  $R$  is the two-dimensional vector

$$\begin{aligned} R_i &= \sum_{j=x,y} d_{ij}(\rho_j - \rho'_j - w_j(z - z')), \quad i = x, y \\ d_{ij} &= \begin{pmatrix} (m_1/m_2)^{1/4} & 0 \\ 0 & (m_2/m_1)^{1/4} \end{pmatrix}. \quad (46) \end{aligned}$$

As  $|\rho| \rightarrow \infty$ , the magnitude of  $R$  goes to infinity, too, and making use of the asymptotic expansion for  $J_0(\bar{k}R)$ <sup>14</sup> we find that (45) may be approximated by

$$\begin{aligned} \lim_{\rho \rightarrow \infty} G^{(+)}(\vec{r}, \vec{r}') &\cong \sum_{\alpha(\text{allowed})} \frac{M}{2\hbar^2} \left( \frac{2i}{\pi K_{\alpha} R} \right)^{1/2} \\ &e^{iK_{\alpha} R} \zeta_{\alpha}(z) \zeta_{\alpha}(z'), \quad (47) \end{aligned}$$

$$K_{\alpha} = [2M(E - \epsilon_{\alpha})/\hbar^2]^{1/2}.$$

The sum over  $\alpha$  is restricted to those subbands for which  $E - \epsilon_{\alpha}$  or  $E_{\alpha_0\hbar_0} - \epsilon_{\alpha}$  is positive. The other subbands yield exponentially decaying out-

going waves and are omitted. One can further expand  $R$  and finally obtain

$$G^{(*)}(\vec{r}, \vec{r}') = \sum_{\alpha} (M/2\hbar^2) (2i/\pi K_{\alpha} \rho_d)^{1/2} \\ \times e^{iK_{\alpha} \rho_d} e^{-i(\vec{w} \cdot \vec{k}_{\alpha}) z} \zeta_{\alpha}(z) \\ \times [e^{-i\vec{k}_{\alpha} \cdot \rho'} e^{i(\vec{w} \cdot \vec{k}_{\alpha}) z'} \zeta_{\alpha}(z')] , \\ \rho_d = [(m_1/m_2)^{1/2} x^2 + (m_2/m_1)^{1/2} y^2]^{1/2} , \quad (48) \\ \vec{k}_{\alpha} = K_{\alpha} [ (m_1/m_2)^{1/2} (x/\rho_d) \hat{x} \\ + (m_2/m_1)^{1/2} (y/\rho_d) \hat{y} ] .$$

By substituting  $\vec{k}_{\alpha}$  into  $E_{\alpha \vec{k}}$  given by (6) it is easily verified that

$$E_{\alpha \vec{k}_{\alpha}} = \epsilon_{\alpha} + \hbar^2 K_{\alpha}^2 / 2M = E = E_{\alpha_0 \vec{k}_0} . \quad (49)$$

Hence, the square-bracketed function in (48) is an eigenfunction of the unperturbed Hamiltonian belonging to  $\alpha$  subband wave vector  $\vec{k}_{\alpha}$  having the same energy as the incident wave. Inserting (48) into (38) we find

$$\psi^{(*)}(\vec{r}) = \phi_0(\vec{r}) + \sum_{\alpha} (e^{iK_{\alpha} \rho_d} / \sqrt{\rho_d}) \zeta_{\alpha}(z) \\ \times e^{-i(\vec{w} \cdot \vec{k}_{\alpha}) z} f_{\alpha \vec{k}_{\alpha}} , \quad (50)$$

where

$$f_{\alpha \vec{k}_{\alpha}} = - (M/2\hbar^2) (2i/K_{\alpha})^{1/2} \\ \times \int d^3r' e^{-i\vec{k}_{\alpha} \cdot \rho'} e^{i(\vec{w} \cdot \vec{k}_{\alpha}) z'} \zeta_{\alpha}(z') \\ \times V(\vec{r}') \psi^{(*)}(\vec{r}') . \quad (51)$$

We now calculate from Eq. (50) the transition probability and scattering cross section from the state  $\alpha_0 \vec{k}_0$  to  $\alpha \vec{k}_{\alpha}$ . They can be determined by comparing the flux of scattered and incident waves. According to the Hamiltonian (1), the flux or particle current density for any wave function  $\psi(r)$  is

$$J_i(\vec{r}) = \sum_j \frac{\hbar}{2i} w_{ij} \left[ \psi^*(\vec{r}) \frac{\partial}{\partial x_j} \psi(\vec{r}) \right. \\ \left. - \left( \frac{\partial}{\partial x_j} \psi^*(\vec{r}) \right) \psi(\vec{r}) \right] . \quad (52)$$

In particular, for the eigenfunctions  $\psi_{\alpha \vec{k}}(\vec{r})$  of the unperturbed Hamiltonian [Eq. (6)],  $J$  only has  $x$  and  $y$  components. Explicitly,

$$J_x(\vec{r}) = (\hbar k_x / 2m_1) |\zeta_{\alpha}(z)|^2 , \\ J_y(\vec{r}) = (\hbar k_y / 2m_2) |\zeta_{\alpha}(z)|^2 , \\ J_z(\vec{r}) = 0 . \quad (53)$$

In deriving (53), the fact that  $w_{12} = w_{13} w_{23} / w_{33}$  has been used. It is more convenient to work with the surface flux  $j_{x,y}(\vec{\rho})$  defined as

$$j_{x,y}(\vec{\rho}) = \int_0^{\infty} dz J_{x,y}(\vec{\rho}, z) . \quad (54)$$

Thus, for the eigenstate ( $\alpha \vec{k}$ ), the surface flux is simply

$$j_x^{\alpha \vec{k}} = \hbar k_x / m_1 , \quad j_y^{\alpha \vec{k}} = \hbar k_y / m_2 , \quad (55)$$

independent of  $\alpha$ . It is noted that the flow of particles, described by the vector  $\vec{j}$ , is different from the direction  $\vec{k}$  because of the anisotropy of the kinetic energy. The incident flux  $j_0$  is given by

$$j_0 = \hbar (k_{0x}^2 / m_1^2 + k_{0y}^2 / m_2^2)^{1/2} . \quad (56)$$

Next, we examine the flux of particles carried by the wave scattered into the  $\alpha$  subband:

$$\Delta \psi_{\alpha}^{(*)}(\vec{r}) = (e^{iK_{\alpha} \rho_d} / \sqrt{\rho_d}) \zeta_{\alpha}(z) \\ \times e^{-i(\vec{w} \cdot \vec{k}_{\alpha}) z} f_{\alpha \vec{k}_{\alpha}} . \quad (57)$$

It also has no  $z$  component, and the leading terms of its  $x$  and  $y$  components are given by

$$j_x^{\alpha \vec{k}_{\alpha}} = (1/\rho_d) (\hbar k_{\alpha x} / m_1) |f_{\alpha \vec{k}_{\alpha}}|^2 , \quad (58)$$

$$j_y^{\alpha \vec{k}_{\alpha}} = (1/\rho_d) (\hbar k_{\alpha y} / m_2) |f_{\alpha \vec{k}_{\alpha}}|^2 .$$

From the definition of  $\vec{k}_{\alpha}$  in Eqs. (48), we see that the scattered flux  $j_{\alpha}$  is parallel to the radius vector  $\vec{\rho}$ :

$$\vec{j}_{\alpha} = \vec{\rho} / \rho = \cos \theta \hat{x} + \sin \theta \hat{y} , \quad (59)$$

which is again different from the direction of  $\vec{k}_{\alpha}$ . We have introduced the angle  $\theta$  as that between the radial vector  $\vec{\rho}$  and the  $x$  axis.

The relations between the various vectors introduced are illustrated in detail in Fig. 1. The relevant quantity to calculate is the particle flux passing through the line segment  $\rho d\theta$  at the angle

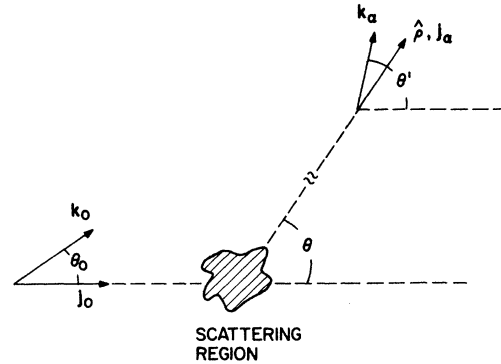


FIG. 1. Incident particle is in state  $\vec{k}_0$  with velocity along  $\vec{j}_0$ . Scattered particle is detected at  $\vec{\rho}$  ( $\hat{\rho} = \vec{\rho}/\rho$ ), and is in state  $\vec{k}_{\alpha}$  with velocity  $\vec{j}_{\alpha}$  which coincides with  $\hat{\rho}$ .

$\theta$ . This is simply equal to

$$\vec{p} d\theta \cdot \vec{j}_\alpha = \left( \frac{\rho}{\rho_d} \right) \hbar \left( \frac{k_{\alpha x}^2}{m_1^2} + \frac{k_{\alpha y}^2}{m_2^2} \right)^{1/2} |f_{\alpha \vec{k}_\alpha}|^2 d\theta$$

or

$$= \frac{d\theta}{[(m_1/m_2)^{1/2} \cos^2 \theta + (m_2/m_1)^{1/2} \sin^2 \theta]^{1/2}} \times \hbar \left( \frac{k_{\alpha x}^2}{m_1^2} + \frac{k_{\alpha y}^2}{m_2^2} \right)^{1/2} |f_{\alpha \vec{k}_\alpha}|^2 \quad (60)$$

upon using the expression for  $\rho_d$  [Eqs. (48)]. The above expression represents the transition probability per unit time of finding the incident particle scattered into the  $\alpha$  subband with surface velocity directed between  $\theta$  and  $\theta + d\theta$ . To obtain the desired transition rate  $dW$  from the state  $(\alpha_0 k_0)$  to  $(\alpha k_\alpha)$ , where  $k_\alpha$  lies between  $\theta'$  and  $\theta' + d\theta'$ , we must express all functions of the angle  $\theta$  in (60) in terms of functions of  $\theta'$ . According to (48) and (59), the angles  $\theta$  and  $\theta'$  are related by

$$\begin{aligned} \vec{k}_\alpha / |\vec{k}_\alpha| &= \cos \theta' \hat{x} + \sin \theta' \hat{y}, \\ \tan \theta' &= (m_2/m_1) \tan \theta. \end{aligned} \quad (61)$$

Then after some algebra we obtain the result

$$\begin{aligned} dW_{\alpha_0 \vec{k}_0 \rightarrow \alpha \vec{k}_\alpha} &= d\theta' \frac{(\hbar k_\alpha / M)}{[(m_2/m_1)^{1/2} \cos^2 \theta' + (m_1/m_2)^{1/2} \sin^2 \theta']} \\ &\times |f_{\alpha \vec{k}_\alpha}|^2 \\ &= d\theta' (\hbar k_\alpha^2 / MK_\alpha) |f_{\alpha \vec{k}_\alpha}|^2, \end{aligned} \quad (62)$$

$$|\vec{k}_\alpha| = \frac{K_\alpha}{[(m_2/m_1)^{1/2} \cos^2 \theta' + (m_1/m_2)^{1/2} \sin^2 \theta']^{1/2}}.$$

This formula can be expressed in a different way by substituting Eq. (51) for  $f_\alpha$  as

$$\begin{aligned} dW_{\alpha_0 \vec{k}_0 \rightarrow \alpha \vec{k}_\alpha} &= d\theta' \frac{M/2\pi \hbar^3}{[(m_2/m_1) \cos^2 \theta' + (m_1/m_2) \sin^2 \theta']} \\ &\times |\langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle|^2 \\ &= d\theta' \left( \frac{k_\alpha}{K_\alpha} \right)^2 \frac{M}{2\pi \hbar^3} |\langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle|^2, \end{aligned} \quad (63)$$

where

$$\begin{aligned} \langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle &= \langle \alpha \vec{k}_\alpha | V | \psi^{(+)} \rangle = t_\alpha(\vec{k}_\alpha) \\ &= \int d^2 p' dz' \xi_\alpha(z') e^{i(\vec{w} \cdot \vec{k}_\alpha) z'} e^{-i\vec{k}_\alpha \cdot \vec{r}'} \\ &\times V(\vec{r}') \psi^{(+)}(\vec{r}') \end{aligned} \quad (64)$$

is what is known as the  $t$ -matrix element [evaluated on the energy shell, i. e.,  $E_{\alpha k} = E (= E_{\alpha_0 k_0})$  or  $k = k_\alpha$ ].<sup>13</sup> A quick way of deriving (63) is to make use of the result of formal scattering theory.<sup>13</sup> The transition probability from the state  $(\alpha_0 k_0)$  to any  $k$  state in the  $\alpha$  subband is given by

$$\begin{aligned} W_{\alpha_0 \vec{k}_0 \rightarrow \alpha} &= (2\pi/\hbar) \int (d^2 k / (2\pi)^2) \\ &\times |\langle \alpha \vec{k} | t | \alpha_0 \vec{k}_0 \rangle|^2 \delta(E_{\alpha \vec{k}} - E) \\ &= (1/2\pi\hbar) \int d\theta' k dk |\langle \alpha \vec{k} | t | \alpha_0 \vec{k}_0 \rangle|^2 \\ &\times \delta \left( \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2} - E \right). \end{aligned} \quad (65)$$

One immediately obtains the partial rate (63) by holding the angle of  $k$  to lie between  $\theta'$  and  $\theta' + d\theta'$ .

The differential cross section for scattering from  $\alpha_0 \vec{k}_0$  to  $\alpha \vec{k}_\alpha$  is obtained by dividing the transition rate per unit angle,  $dW/d\theta'$ , by the magnitude of the incident flux,  $j_0$ . Therefore, according to (56) we have

$$\begin{aligned} \frac{d\sigma_\alpha}{d\theta'} &= \left[ \frac{(m_2/m_1)^{1/2} \cos^2 \theta_0 + (m_1/m_2)^{1/2} \sin^2 \theta_0}{(m_2/m_1) \cos^2 \theta_0 + (m_1/m_2) \sin^2 \theta_0} \right]^{1/2} \\ &\times \frac{k_\alpha^2}{K_0 K_\alpha} |f_{\alpha \vec{k}_\alpha}|^2, \end{aligned} \quad (66)$$

where  $\theta_0$  is the angle for  $\vec{k}_0$  and  $K_0$  is defined similar to  $K_\alpha$ , i. e.,

$$\vec{k}_0 / |\vec{k}_0| = \cos \theta_0 \hat{x} + \sin \theta_0 \hat{y}, \quad (67)$$

$$K_0 = [2M(E - \epsilon_0)/\hbar^2]^{1/2}.$$

The transition probability or scattering cross section is known once the scattering amplitude  $f_{\alpha \vec{k}_\alpha}$  or the  $t$ -matrix element  $t_\alpha(\vec{k}_\alpha)$  is determined. A perturbation series in the potential  $V$  for  $t_\alpha(\vec{k}_\alpha)$  is obtained by iterating the exact outgoing wave  $\psi^{(+)}(\vec{r})$  according to Eq. (38). The first Born approximation corresponds to the first step in the iteration, that is,  $\psi^{(+)}(\vec{r})$  is replaced by the incident wave  $\phi_0(r)$ , yielding the following familiar result

$$\begin{aligned} \langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle &= \langle \alpha \vec{k}_\alpha | V | \alpha_0 \vec{k}_0 \rangle \\ &= V^{\alpha \alpha_0}(\vec{k}_\alpha - \vec{k}_0). \end{aligned} \quad (68)$$

Putting this expression into (63) we obtain

$$\frac{dW}{d\theta'}_{\alpha_0 \vec{k}_0 \rightarrow \alpha \vec{k}_\alpha} = \left( \frac{k_\alpha}{K_\alpha} \right)^2 \frac{M}{2\pi \hbar^3} |V^{\alpha \alpha_0}(\vec{k}_\alpha - \vec{k}_0)|^2. \quad (69)$$

#### B. Scattering of Many Impurities

In Sec. IIIA we considered only the scattering



by one impurity center. In the sample there are many such centers, consisting of the almost uniformly distributed negatively charged acceptor centers in the depletion layer and the charged impurities in the oxide localized near the interface. We denote their positions by  $\vec{r}_i = \vec{\rho}_i + z_i$ . The total  $t$ -matrix element for scattering from the state  $\alpha_0 \vec{k}_0$  to  $\alpha \vec{k}_\alpha$  is

$$\langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle = \langle \alpha \vec{k}_\alpha | \sum_i V^i | \psi^{(+)}, \alpha_0 \vec{k}_0 \rangle, \quad (70)$$

where  $V^i$  represents the screened potential of  $i$ th impurity and  $|\psi^{(+)}, \alpha_0 \vec{k}_0\rangle$  is the outgoing wave function arising from the incident state  $(\alpha_0 \vec{k}_0)$  in the presence of the total potential  $V = \sum_i V^i$ . To proceed, we make the usual systematic expansion of (70) in terms of the  $t$  matrices for the individual scattering centers.<sup>13</sup> Retaining only the first two terms, we obtain

$$\begin{aligned} \langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle &= \sum_i \langle \alpha \vec{k}_\alpha | t^i | \alpha_0 \vec{k}_0 \rangle \\ &\quad - \sum_{i \neq j} \sum_{\alpha' \vec{k}'} \langle \alpha \vec{k}_\alpha | t^i | \alpha' \vec{k}' \rangle \\ &\quad \times G_{\alpha'}^{(+)}(\vec{k}') \langle \alpha' \vec{k}' | t^j | \alpha_0 \vec{k}_0 \rangle, \\ G_{\alpha'}^{(+)}(\vec{k}') &= 1/[E_{\alpha'}(\vec{k}') - E_{\alpha_0}(\vec{k}_0) - i\epsilon]. \end{aligned} \quad (71)$$

The quantity  $\langle \alpha \vec{k}_\alpha | t^i | \alpha_0 \vec{k}_0 \rangle$  is the  $t$  matrix due to the single potential  $V^i$ . By translational symmetry in the  $(x, y)$  direction, it is readily shown that

$$V^i(\vec{r}) = V(\vec{\rho} - \vec{\rho}_i; z_i),$$

$$\langle \alpha \vec{k}_\alpha | t^i | \alpha_0 \vec{k}_0 \rangle = e^{-i(\vec{k}_\alpha - \vec{k}_0) \cdot \vec{\rho}} \langle \alpha \vec{k}_\alpha | t^i | \alpha_0 \vec{k}_0 \rangle, \quad (72)$$

where  $t^i$  represents the  $t$  matrix for the potential resulting from a translation of  $V^i$  to the origin in the  $(x, y)$  plane ( $\rho = 0$ ). This is the quantity we have calculated in Sec. III C.

The quantity we wish to obtain is the transition probability, or equivalently

$$\langle |\langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle|^2 \rangle_{\text{av}}, \quad (73)$$

where  $\langle \rangle$  denotes an averaging over the positions of the impurity sites according to some distribu-

tion law. If the impurities are randomly placed or uncorrelated and multiple scattering is neglected, the total transition probability will be simply given by a sum of the individual transition probabilities, i. e.,

$$\begin{aligned} \langle |\langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle|^2 \rangle_{\text{av}} &\approx \langle \sum_i |\langle \alpha \vec{k}_\alpha | t^i | \alpha_0 \vec{k}_0 \rangle|^2 \rangle_{\text{av}} \\ &= N_A \int_0^d dz \langle |\langle \alpha \vec{k}_\alpha | t^z | \alpha_0 \vec{k}_0 \rangle|^2 \rangle \\ &\quad + N_{\text{int}} |\langle \alpha \vec{k}_\alpha | t^{(-)} | \alpha_0 \vec{k}_0 \rangle|^2, \end{aligned} \quad (74)$$

where  $d$  is thickness of the depletion layer,  $N_A$  is the concentration of acceptors ( $N_A \lesssim 10^{16} \text{ cm}^{-3}$ ), and  $N_{\text{int}}$  is the number of charged impurities per unit area in the oxide at the interface ( $N_{\text{int}} \sim 10^{11} \text{ cm}^{-2}$ ). In arriving at (73), we have assumed that the surface scattering centers are identical and that the variation of their positions in the  $z$  direction is small. Thus  $t^{(-)}$  represents the scattering amplitude for one surface impurity at the origin ( $\vec{\rho} = 0, z = 0$ ).

We now consider two effects which lead to corrections to the simple result given in (74). The first is the interference of the scattered waves from different impurities when their positions are correlated. For the consideration of this effect, one need only keep the first term in (71) of the total  $t$  matrix. The second term in (71) describes multiple scattering and will be dealt with later. In order to perform the averaging indicated by (73), a very simple model of correlation among the impurities will be used. We assume that the positions of the surface impurities ( $N_{\text{int}}$ ) and the impurities in the bulk, i. e., the acceptor centers in the depletion layer, are not correlated. Second, we assume that there is still no correlation between the bulk impurities when their  $z$  coordinates are separated by a distance greater than a certain length  $\Delta$ . Finally, the correlation between the surface impurities and the correlation between the bulk impurities which are located inside a slab of thickness  $\Delta$  are taken to be of the hard-core type, i. e., the only restriction is that no two impurities can be found within a distance  $\rho_0$  of each other. Under these assumptions we readily obtain the result

$$\langle |\langle \alpha \vec{k}_\alpha | t | \alpha_0 \vec{k}_0 \rangle|^2 \rangle_{\text{av}} = N_A [1 - N_A \nu(k_{\alpha 0}) \Delta] \int_0^d dz \langle |\langle \alpha \vec{k}_\alpha | t^z | \alpha_0 \vec{k}_0 \rangle|^2 \rangle + N_{\text{int}} [1 - N_{\text{int}} \nu(k_{\alpha 0})] |\langle \alpha \vec{k}_\alpha | t^{(-)} | \alpha_0 \vec{k}_0 \rangle|^2,$$

$$\nu(k_{\alpha 0}) = (2\pi\rho_0/k_{\alpha 0}) J_1(k_{\alpha 0}\rho_0), \quad k_{\alpha 0} = |\vec{k}_\alpha - \vec{k}_0|.$$

The quantity  $\nu(k_{\alpha 0})$  is just the Fourier transform of the excluded area  $\rho \leq \rho_0$ . In the present case  $k_{\alpha 0}$  is of the order of  $k_F \sim 2 \times 10^6 \text{ cm}^{-1}$  for ( $N_{\text{inv}} \sim 10^{12} \text{ cm}^{-2}$ ),  $N_A \sim 10^{16} \text{ cm}^{-3}$ , and  $N_{\text{int}} \sim 10^{11} \text{ cm}^{-2}$ . Taking  $\Delta$  and  $\rho_0$  to be roughly equal to  $20 \text{ \AA}$ , one finds that the reduction of the transition probability due to interference is negligible for the bulk impurities and is about a few percent for the surface impurities.

The other effect which leads to corrections to the simple result (74) is multiple scattering. It describes processes in which the electron scatters from the initial to the final state via intermediate states involving at least two different impurities. The terms in the  $t$  matrix responsible for these events are the second- (and higher-order terms) in the expansion in (71). We will now insert (71)

into (73) and perform the indicated average. The contribution by the first term in (71) alone was calculated yielding the result shown in Eqs. (75). The leading correction due to multiple scattering comes from the averaging of the product of the first and second terms of (71):

$$-\sum_i \sum_{i \neq j} \sum_{\alpha' \vec{k}'} \langle \alpha \vec{k}_\alpha | t^i | \alpha_0 \vec{k}_0 \rangle \\ \times \langle \alpha \vec{k}_\alpha | t^j | \alpha' \vec{k}' \rangle G_{\alpha'}^{(+)}(\vec{k}') \\ \times \langle \alpha' \vec{k}' | t^j | \alpha_0 \vec{k}_0 \rangle \quad . \quad (76)$$

We shall ignore the correlation of three different impurity centers and therefore only retain the terms  $l=i$  or  $j$ . Using the same model to describe the correlation as before one arrives at the expression

$$N_A^2 \Delta \int_0^d dz \langle \alpha \vec{k}_\alpha | t^z | \alpha_0 \vec{k}_0 \rangle^* \sum_{\alpha' \vec{k}'} \{ \langle \alpha \vec{k}_\alpha | t^z | \alpha' \vec{k}' \rangle G_{\alpha'}^{(+)}(\vec{k}') \langle \alpha' \vec{k}' | t^z | \alpha_0 \vec{k}_0 \rangle [\nu(\vec{k}' - \vec{k}_0) + \nu(\vec{k}' - \vec{k}_d)] \} \\ + N_{\text{int}}^2 \langle \alpha \vec{k}_\alpha | t^{(-)} | \alpha_0 \vec{k}_0 \rangle^* \sum_{\alpha' \vec{k}'} \{ \langle \alpha \vec{k}_\alpha | t^{(-)} | \alpha' \vec{k}' \rangle G_{\alpha'}^{(+)}(\vec{k}') \langle \alpha' \vec{k}' | t^{(-)} | \alpha_0 \vec{k}_0 \rangle \\ \times [\nu(\vec{k}' - \vec{k}_0) + \nu(\vec{k}' - \vec{k}_\alpha)] \} + (\text{c. c.}) \quad (77)$$

The indicated summation and integration will be carried out in an approximate way to obtain a qualitatively meaningful result. The important fact to realize is that the Green's function is large when  $\alpha = \alpha_0$  and  $|k'|$  near  $k_0$  [ $E_{\alpha'}(k') \sim E_{\alpha_0}(k_0)$ ] and accordingly one replaces the slowly varying functions inside the integral by some appropriately chosen average values.

The final result is

$$\sim (N_A \int_0^d dz |\langle \alpha \vec{k}_\alpha | t^z | \alpha_0 \vec{k}_0 \rangle|^2) N_A \nu(k_0) \\ \times \Delta [ |t| (2M/\pi \hbar^2) \ln(k_c/k_0) ] \\ + (N_{\text{int}} |\langle \alpha \vec{k}_\alpha | t^{(-)} | \alpha_0 \vec{k}_0 \rangle|^2) \\ \times N_{\text{int}} \nu(k_0) [ |t^{(-)}| (2M/\pi \hbar^2) \ln(k_c/k_0) ], \quad (78)$$

where  $|t|$  and  $|t^{(-)}|$  are some typical values of the  $t$ -matrix elements;  $M$  is a mass which may be taken as  $(m_1 m_2)^{1/2}$ , and  $k_c$  ( $> k_0$ ) is the high-momentum cutoff of the  $k'$  integration due to either the  $t$ -matrix element or the correlation function  $\nu$ . It is observed that the correction factor on the transition probability due to multiple scattering involves an extra ratio

$$r = |t| (2M/\pi \hbar^2) \ln(k_c/k_0) \quad (79)$$

so compared to that due to interference [see Eqs. (75)]. For charged impurity scattering  $|t| \sim 4\pi e^2/\kappa s$ , where  $s$  is the screening length given by (34). Then putting  $k_0 \sim 1/\rho_0 \sim \frac{1}{2} 10^7$ ,  $k_0 \sim k_F \sim 2 \times 10^6$ ,  $r$  is found to be of order unity. Thus the leading correction due to multiple scattering has the same magnitude as the correction due to interference. The next-order contribution to the transition probability due to multiple scattering is readily estimated to be similar to (78) with  $r^2$  instead of  $r$ . This leads to an interesting observation. If  $r$  is larger than unity because  $k_0$  ( $k_F$ ) is much smaller than  $k_c$ , the successive terms in the perturbation expansion in multiple scattering will diverge. In this case, we must go beyond perturbation calculation, for example, and sum selectively an infinite number of terms to obtain any meaningful result.<sup>15</sup>

### C. Surface Conductivity

Our next task is the calculation of the surface conductivity of the electrons in the inversion layer due to impurity scattering. The quantity to determine first is the electronic current in a static electric field parallel to the surface. Since intervalley scattering has been neglected, the current is equal to the sum of the contribution from each val-

ley. Thus, it suffices to consider one valley at a time. To first order in the electric field  $\vec{E}$ , we have

$$J_i^v = \sum_j \sigma_{ij}^v E_j, \quad (i, j) = (x, y) \quad (80)$$

$$\sigma_{ij}^{\text{tot}} = \sum_v \sigma_{ij}^v.$$

The conductivity tensor  $\sigma_{ij}^v$  for any valley  $v$  is, in general, not diagonal because of the particular orientation of its constant-energy ellipsoid. But for our purpose we shall again choose the coordinate system such that  $w_{12}^v = w_{13}^v w_{23}^v / w_{33}^v$ , in which  $\sigma_{ij}^v$  is therefore diagonal. However, the diagonal matrix elements  $\sigma_{xx}$  and  $\sigma_{yy}$  (we shall drop the valley index  $v$ ) are still not equal because the effective masses  $m_1$  and  $m_2$  defined in Eq. (42) are different.

The conductivity is calculated in the usual manner by making use of the electron Boltzmann equation.<sup>16</sup> Denoting the distribution function of the electron in the  $\alpha$  subband and wave vector  $\vec{k}$  by  $f_\alpha(\vec{k})$  (for electrons in the valley  $v$  under consideration), we have

$$-\frac{e}{\hbar} \vec{E} \cdot \frac{\partial}{\partial \vec{k}} f_\alpha(\vec{k}) = - \sum_{\alpha', \vec{k}'} P_{\alpha', \vec{k}', \alpha \vec{k}} f_\alpha(\vec{k}) + \sum_{\alpha', \vec{k}'} P_{\alpha \vec{k}, \alpha', \vec{k}'} f_{\alpha'}(\vec{k}'), \quad (81)$$

where  $\vec{E}$  is the electric field and  $P_{\alpha', \vec{k}', \alpha \vec{k}}$  is the transition probability per unit time from the state  $(\alpha, \vec{k})$  to the state  $(\alpha', \vec{k}')$ . According to the discussions in the Sec. III B, it is given by

$$P_{\alpha', \vec{k}', \alpha \vec{k}} = (2\pi/\hbar) \langle |\langle \alpha \vec{k} | t | \alpha' \vec{k}' \rangle|^2 \rangle_{\text{av}} \times \delta(E_{\alpha'}(\vec{k}') - E_\alpha(\vec{k})), \quad (82)$$

$$P_{\alpha', \vec{k}', \alpha \vec{k}} = P_{\alpha \vec{k}, \alpha', \vec{k}'}, \quad .$$

In thermal equilibrium ( $\vec{E} = 0$ ) the distribution function is the Fermi function,

$$f_\alpha^0(\vec{k}) = 1/(e^{\beta(E_\alpha(\vec{k}) - \zeta)} + 1) \quad (83)$$

$\zeta$  = Fermi energy .

For a small field, we are interested in calculating the correction to  $f^0$  that is linear in the field strength. Accordingly, we put

$$f_\alpha(\vec{k}) = f_\alpha^0(\vec{k}) + g_\alpha(\vec{k}) \quad (84)$$

and deduce the following equation for  $g$ , the deviation from equilibrium:

$$e[\vec{E} \cdot \vec{j}(\vec{k})] S_\alpha^0(\vec{k}) = - \sum_{\alpha', \vec{k}'} P_{\alpha', \vec{k}', \alpha \vec{k}} [g_\alpha(\vec{k}) - g_{\alpha'}(\vec{k}')] , \quad (85)$$

where  $S_\alpha^0(\vec{k}) = \beta f_\alpha^0(\vec{k}) [1 - f_\alpha^0(\vec{k})] = S^0(E_\alpha(\vec{k}))$  ,

$$\vec{j}(\vec{k}) = \frac{1}{\hbar} \frac{\partial}{\partial \vec{k}} E_\alpha(\vec{k}) = \frac{\hbar}{m_1} k_x \hat{x} + \frac{\hbar}{m_2} k_y \hat{y} . \quad (86)$$

It is well known that only for very special cases can we solve the integral equation (85) analytically.<sup>16</sup> One such simple situation occurs when  $m_1 = m_2 = m$  so that  $\vec{j}(\vec{k}) = (\hbar/m)\vec{k}$  and the transition probability  $P_{\alpha', \vec{k}', \alpha \vec{k}}$  depends only on the angle between  $\vec{k}$  and  $\vec{k}'$  [and of course on the energy  $E_\alpha(\vec{k}) = E_\alpha(\vec{k}')$ ]. Then we readily find the solution

$$g_\alpha(\vec{k}) = -e \tau_\alpha(E_\alpha(\vec{k})) [\vec{E} \cdot (\hbar/m)\vec{k}] S^0(E_\alpha(\vec{k})) . \quad (87)$$

The relaxation time  $\tau_\alpha$  introduced in (87) is only a function of the energy  $E_\alpha(\vec{k})$  and is determined by

$$\tau_\alpha P_\alpha - \sum_{\alpha' \neq \alpha} P_{\alpha \alpha'} \tau_{\alpha'} = 1 , \quad (88)$$

where

$$P_\alpha(\vec{k}) = P_\alpha(E_\alpha(\vec{k})) = \frac{2\pi}{\hbar} \int \frac{d^2 k'}{(2\pi)^2} \langle |\langle \alpha \vec{k} | t | \alpha \vec{k}' \rangle|^2 \rangle_{\text{av}} (1 - \cos\phi) \delta(E_\alpha(\vec{k}) - E_\alpha(\vec{k}')) + \sum_{\alpha' \neq \alpha} \frac{2\pi}{\hbar} \int \frac{d^2 k'}{(2\pi)^2} \langle |\langle \alpha' \vec{k}' | t | \alpha \vec{k} \rangle|^2 \rangle_{\text{av}} \delta(E_\alpha(\vec{k}) - E_{\alpha'}(\vec{k}')) , \quad P_{\alpha \alpha'}(\vec{k}) = P_{\alpha \alpha'}(E_\alpha(\vec{k})) = \frac{2\pi}{\hbar} \frac{k_{\alpha'}}{k} \int \frac{d^2 k'}{(2\pi)^2} \langle |\langle \alpha' \vec{k}' | t | \alpha \vec{k} \rangle|^2 \rangle_{\text{av}} \cos\phi \delta(E_\alpha(\vec{k}) - E_{\alpha'}(\vec{k}')) , \quad \cos\phi = \vec{k} \cdot \vec{k}' / |\vec{k}| |\vec{k}'| . \quad (89)$$

The electronic current is immediately obtained from (87) (we put back the valley index  $v$  to avoid confusion<sup>6</sup>):

$$\vec{J}^v = -2e \sum_{\alpha \vec{k}} (\hbar/m^v) \vec{k} g_\alpha^v(\vec{k}) . \quad (90)$$

Upon using the fact that the electron energy  $E_\alpha(k)$

is isotropic, we finally find

$$\begin{aligned} \vec{J}^v &= \sigma^v \vec{E}, \\ \sigma^v &= \frac{2e^2}{m^v} \sum_{\alpha} \int \frac{d^2k}{(2\pi)^2} \tau_{\alpha}^v(E_{\alpha}^v(\vec{k})) [E_{\alpha}^v(\vec{k}) - \epsilon_{\alpha}^v] S^0(E_{\alpha}^v(\vec{k})). \end{aligned} \quad (91)$$

At zero temperature,

$$S^0(E_{\alpha}^v(\vec{k})) = \delta(E_{\alpha}^v(\vec{k}) - \xi^0),$$

where  $\xi^0$  is the Fermi energy. Then, the conductivity tensor, which is just a constant matrix, is simply

$$\sigma^v = (e^2/\pi \hbar^2) \sum_{\alpha(\epsilon_{\alpha}^v < \xi^0)} \tau_{\alpha}^v(\xi^0) (\xi^0 - \epsilon_{\alpha}^v); \quad (92)$$

the parameter  $\xi^0$  is determined by the total number of electrons in the inversion layer,

$$N_{\text{inv}} = 2 \sum_{\nu} \sum_{\alpha(\epsilon_{\alpha}^v < \xi^0)} \frac{m^v}{2\pi \hbar^2} (\xi^0 - \epsilon_{\alpha}^v). \quad (93)$$

In our present case the electron energy  $E_{\alpha}^v(\vec{k})$  is not isotropic, so  $\vec{j}^v(\vec{k})$  is not parallel to  $\vec{k}$ . Furthermore  $P_{\alpha\vec{k},\alpha'\vec{k}'}$  has much more complicated angular dependence than the example considered above. However it is beyond the scope of this paper to examine the various approximation schemes one can use to calculate  $g_{\alpha}^v(\vec{k})$ .<sup>17</sup> We shall simply assert that the following expression for  $g_{\alpha}^v(\vec{k})$ , corresponding to a reasonable generalization of the previous result for the isotropic case, is an adequate approximation to the exact solution

$$g_{\alpha}^v(\vec{k}) = -e \tau_{\alpha}^v(E_{\alpha}^v(\vec{k})) [\vec{E} \cdot \vec{j}^v(\vec{k})] S^0(E_{\alpha}^v(\vec{k})), \quad (94)$$

where  $\tau_{\alpha}^v$  is determined by an equation similar to (88), namely,

$$\tau_{\alpha}^v \bar{P}_{\alpha}^v - \sum_{\alpha' \neq \alpha} \bar{P}_{\alpha\alpha'}^v \tau_{\alpha'}^v = 1. \quad (95)$$

The rates  $\bar{P}_{\alpha}^v$  and  $\bar{P}_{\alpha\alpha'}^v$  are essentially averages of  $P_{\alpha}^v$  and  $P_{\alpha\alpha'}^v$  over the constant-energy surface in  $k$  space defined by

$$\hbar^2 k_x^2 / 2m_1^v + \hbar^2 k_y^2 / 2m_2^v = E_{\alpha}^v(\vec{k}) - \epsilon_{\alpha}^v = E - \epsilon_{\alpha}^v.$$

Explicitly, we have

$$\begin{aligned} \bar{P}_{\alpha}^v &= \int_0^{2\pi} d\theta \left( \frac{\cos^2 \theta}{m_1^v} + \frac{\sin^2 \theta}{m_2^v} \right)^{-1} P_{\alpha}^v(\vec{k}) / \\ &\int_0^{2\pi} d\theta \left( \frac{\cos^2 \theta}{m_1^v} + \frac{\sin^2 \theta}{m_2^v} \right)^{-1}, \\ k_x &= k^v \cos \theta, \quad k_y = k^v \sin \theta, \\ k^v &= \frac{1}{\hbar} \left( \frac{2(E - \epsilon_{\alpha}^v)}{\cos^2 \theta / m_1^v + \sin^2 \theta / m_2^v} \right)^{1/2}, \end{aligned} \quad (96)$$

and similarly for  $\bar{P}_{\alpha\alpha'}^v$ . The prime on  $P_{\alpha}^v(\vec{k})$  inside the integral in (96) is to denote that the cosine of the angle  $\phi$  between  $\vec{k}$  and  $\vec{k}'$  [see Eq. (86)] must be replaced by the cosine of the angle  $\phi^v$  between  $\vec{j}^v$

$\times(\vec{k})$  and  $\vec{j}^v(\vec{k}')$ :

$$\cos \phi^v = \vec{j}^v(\vec{k}) \cdot \vec{j}^v(\vec{k}') / |\vec{j}^v(\vec{k})| |\vec{j}^v(\vec{k}')|. \quad (97)$$

The electronic current for the distribution (94) is

$$\begin{aligned} J_i^v &= -2e \sum_{\alpha\vec{k}} j_i^v(\vec{k}) g_{\alpha}^v(\vec{k}) \\ &= \sum_j (2e^2 \sum_{\alpha\vec{k}} \tau_{\alpha}^v(E_{\alpha}^v(\vec{k})) j_i^v(\vec{k}) j_j^v(\vec{k}) S^0(E_{\alpha}^v(\vec{k})) E_j). \end{aligned} \quad (98)$$

From (98) one immediately obtains the conductivity tensor

$$\sigma_{ij}^v = 2e^2 \sum_{\alpha\vec{k}} \tau_{\alpha}^v(E_{\alpha}^v(\vec{k})) j_i^v(\vec{k}) j_j^v(\vec{k}) S^0(E_{\alpha}^v(\vec{k})). \quad (99)$$

The observed conductivity is of course given by the sum of the above expressions over all the valleys.

#### IV. CONCLUDING REMARKS

We have considered two aspects of the problem of  $n$ -type inversion layers in which the electrons occupy several discrete electric subbands. The first is the screening of external potentials, which is found to be conveniently described by a matrix dielectric function. It is found that the extent of screening depends only weakly on the electron concentration, unlike the situation in the bulk. The second topic studied was the problem of scattering by charged impurities and their contribution to the surface conductivity. Explicit formulas for the scattering cross sections with intersubband transitions in the general case of nonisotropic constant energy surfaces were calculated. The magnitudes of the effects of interference and multiple scattering which are present when there are many scattering centers were estimated. For the concentrations of impurities usually encountered these corrections amount to a few percent. Finally a system of coupled Boltzmann's equations for the distribution functions of the electrons in different subbands was solved exactly for the isotropic case and approximately for the nonisotropic case to obtain the surface conductivity (tensor).

There are several important aspects of the problem which have not been treated here. First of all, there is the interesting question of the electrons in the electric subband entering into bound states of the screened charge impurities. If this happens, motions along the surface will also be quantized. The condition for the formation of such a bound state is much easier to satisfy than in the bulk. If these bound states exist, then at low enough temperatures many electrons will be trapped and this freezing-out phenomenon may lead to drastic changes in the surface mobility.<sup>18</sup> These questions are currently being investigated by the authors. Second, in regard to surface transport

properties, there are other scattering mechanisms which need to be considered. It is clear that phonon scattering will become important at high temperature. Several authors have studied scattering by surface phonons.<sup>19</sup> A preliminary calculation shows that the bulk-phonon scattering is at least as important as the surface-phonon scattering. Recent experimental data at high electron concentration and low temperature show a mobility that is independent of impurity concentration but is rapidly decreasing with gate voltage or electron concentration. This suggests surface-roughness scattering as a possible candidate for the dominating mechanism, because the subband wave functions of the electrons  $\zeta(z)$  are being squeezed

closer to the interface. A calculation based on a simple model for the surface roughness yields a result which agrees well with the experimental data.<sup>20</sup> The bulk-phonon scattering calculation and the surface-roughness scattering calculation will be reported in a subsequent paper.

#### ACKNOWLEDGMENTS

The authors wish to thank Dr. F. Stern for drawing our attention to this problem and for many helpful discussions during the course of the work. Thanks are due to A. Fowler for making available to us new and unpublished experiment results. Several conversations with Dr. T. D. Schultz have also proved to be very valuable.

\*Present address: Harvard College, Cambridge, Mass. 02138.

<sup>1</sup>The phrase "electric quantum limit" was used in Ref. 2 to designate the case when only the lowest electric subband is occupied, which, strictly speaking, can only occur at zero temperature.

<sup>2</sup>F. Stern and W. E. Howard, *Phys. Rev.* **163**, 816 (1967).

<sup>3</sup>It has been proved by D. Jepsen and T. D. Schultz (private communication) that a bound state always exists for an arbitrary attractive potential in two dimensions.

<sup>4</sup>A. B. Fowler (private communication).

<sup>5</sup>W. Kohn, in *Solid State Physics*, Vol. 5, edited by F. Seitz and D. Turnbull (Academic, New York, 1957), p. 257.

<sup>6</sup>The factor of 2 is for spin.

<sup>7</sup>If there are donor impurity atoms in the depletion layer, one should replace  $N_A$  by  $N_A - N_D$ .

<sup>8</sup>See, for example, D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1963), Sec. 3.4. If the external potential oscillates with a frequency  $\omega$ , i. e.,

$$V_{\text{ext}}(r) \rightarrow V_{\text{ext}}(r, \omega)e^{-i\omega t},$$

the induced charge density will become  $\rho_{\text{ind}}(r, \omega)e^{-i\omega t}$ . In an isotropic medium,  $\rho_{\text{ind}}(r, \omega)$  is simply given by expression (11) except that the factor  $i\epsilon$  is replaced by  $+i\epsilon$ . On the other hand, in a nonisotropic medium like the present system there is an extra contribution due to the existence of an induced transverse vector potential  $A$ , and the result is a much more complicated expression.

<sup>9</sup>This is the well-known result of the electrostatic potential obtained by the image-charge method. See any book on electrostatic problems, for example, J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962).

<sup>10</sup>F. Stern, *Phys. Rev. Letters* **18**, 546 (1967).

<sup>11</sup>See, for example, Ref. 6.

<sup>12</sup>This form has been used in Ref. 2 for variational calculations.

<sup>13</sup>See, for example, A. Messiah, *Quantum Mechanics*, Vol. II (Wiley, New York, 1962), Ch. XIX.

<sup>14</sup>For a quick reference of the properties of Bessel functions, see W. Magnus and Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea, New York, 1954).

<sup>15</sup>A review on multiple scattering theory and nonperturbation approximation methods necessary at high concentration of scattering centers may be found in M. Lax, *Rev. Mod. Phys.* **23**, 287 (1951). Currently, new methods are developed to treat multiple scattering in alloys; for example, see the coherent-potential approximation developed by P. Soven, *Phys. Rev.* **178**, 1136 (1969).

<sup>16</sup>See, for example, J. M. Ziman, *Electrons and Phonons* (Oxford U. P., London, 1960), Chap. VII.

<sup>17</sup>For example, the variational principle introduced by Sondheimer described in Ref. 16.

<sup>18</sup>The surface mobility at low temperature and in low-mobility samples shows an exponential dependence on the inverse of the temperature with a relatively constant activation energy which changes with electron concentrations; see F. F. Fang and A. B. Fowler, *Phys. Rev.* **169**, 619 (1968). The exact origin of this behavior is not known but may be connected with the freezing out of mobile electrons in surface bound states. See Ref. 2 for some discussion.

<sup>19</sup>S. Kawaji (unpublished).

<sup>20</sup>R. F. Greene has considered charged bumps scattering at the surface and obtained a mobility that decreases with electron concentration but is much lower than the experimentally observed value [see Proceedings of the Battelle Symposium on Molecular Processes at Solid Surface, Kronberg, Germany, 1968 (unpublished)].