Balance-equation analysis of linear and nonlinear electronic transport in quasi-two-dimensional quantum-well superlattices

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(Received 15 October 1985; revised manuscript received 14 February 1986)

A non-Boltzmann balance-equation approach to linear and nonlinear dc steady-state electronic transport in a type-I superlattice (which is composed of infinitely many periodically arranged finite-width quantum wells) is developed in the presence of an electric field parallel to the superlattice planes. The method is based on a separation of the parallel motion of the center of mass from the relative motion of the electron system. The Coulomb interactions between intralayer and interlayer carriers are naturally built in via the electron density-density correlation function of the superlattice system. The force and energy balance equations obtained are applied to the calculation of the Ohmic mobilities limited by remote and background impurity scatterings and by acoustic and polar optical-phonon scatterings in GaAs-$Al_xGa_{1-x}As$ superlattices. The nonlinear mobility and electron temperature are numerically calculated as functions of drift velocity, including all the above-mentioned scattering mechanisms and the full effect of carrier-carrier Coulomb interaction within the framework of the random-phase approximation. The dependence of transport on the geometrical parameters of the superlattice is discussed.

I. INTRODUCTION

Semiconductor superlattices, first proposed by Esaki and Tsu,[1] have become a central focus in the current development of microstructure science and technology. Modulation doping in semiconductors and steady improvements in thin-film techniques have made it possible to produce high-quality periodic multilayer systems composed of alternating ultrathin layers of different semiconducting materials with similar lattice structure and matching lattice parameters. Such multilayer heterostructure systems of GaAs-$Al_xGa_{1-x}As$ and other semiconductor combinations[2] have been shown to have very high carrier mobilities due to the separation of the mobile charge carriers from the ionized dopants.[3] Many aspects of the physics of such semiconductor superlattices have been extensively studied in the past several years.[4] Theoretical investigations of electron transport, however, were focused mainly on single heterojunction structures. An electron-transport theory pertinent to a superlattice, particularly a nonlinear theory, is still not available at this time, and we therefore address this matter here.

It is well known that the Coulomb interaction between carriers in a two-dimensional (2D) system has an important effect on their transport properties. For a closely packed multilayer system, such an effect is expected to be even more important because of the couplings between interlayer carriers and the carrier scatterings by the charged impurities in different layers. These effects should be taken into full account in establishing a transport theory for superlattices. Recently, a non-Boltzmann balance-equation approach was developed by Lei and Ting[5] to describe nonlinear electronic transport for electron-impurity-phonon systems in the presence of a uniform electric field. The role of the electron-electron interaction is fundamentally built into the theory via the electron density-density correlation function of the system, and the associated screening and nonlinear descreening phenomena are naturally included. This formulation has been proven to be useful and convenient for studying linear and high-field steady-state transport in both the 3D and 2D cases.[6,7] The same method will be employed in this paper to discuss the electron transport, especially nonlinear transport, for a type-I superlattice in the presence of a constant uniform electric field.

II. HAMILTONIAN

The model we shall use for the type-I superlattice consists of an infinite number of periodically arranged quantum wells of width a, and d is the spatial period or distance between two adjacent layer centers. In the effective-mass approximation the electron system can be described generally by the following Hamiltonian:[8]

$$H=\sum_i\left[\frac{\mathbf{p}_i^2}{2m}+\frac{p_{zi}^2}{2m_z}+U(z_i)\right]+\sum_{\substack{i,j\\ i<j}}V(\mathbf{r}_i-\mathbf{r}_j,z_i,z_j)\,, \quad (1)$$

where $\mathbf{p}_i=(p_{xi},p_{yi})$ and $\mathbf{r}_i=(x_i,y_i)$ are the two-dimensional momentum and coordinate of the ith electron along the layer plane and p_{zi} and z_i are those perpendicular to the interface; m and m_z are, respectively, the electron-band effective mass parallel and perpendicular to the plane; $U(z)$ is the potential reflecting the superlattice structure; the last term is the electron-electron interaction. When a uniform electric field is applied parallel to the plane, the electronic transport, or the motion of the center of mass of the electron system, takes place only within the plane. Therefore, it is convenient to introduce two-

dimensional center-of-mass variables $\mathbf{P}=(P_x,P_y)$ and $\mathbf{R}=(X,Y)$:

$$\mathbf{P}=\sum_i \mathbf{p}_i,\quad \mathbf{R}=\frac{1}{N}\sum_i \mathbf{r}_i\ , \tag{2}$$

and two-dimensional relative electron variables

$$\mathbf{p}_i'=\mathbf{p}_i-\frac{1}{N}\mathbf{P},\quad \mathbf{r}_i'=\mathbf{r}_i-\mathbf{R}\ , \tag{3}$$

where N is the total number of electrons (normalized to unit area). In terms of these variables the Hamiltonian of the electron system in the presence of an electric field $\mathbf{E}$ parallel to the layer plane, can be written as the sum of a 2D center-of-mass part H_c and a relative part H_e, with

$$H_c=\frac{\mathbf{P}^2}{2Nm}-Ne\mathbf{E}\cdot\mathbf{R}\ , \tag{4}$$

and H_e is also expressed by Eq. (1) but with $\mathbf{p}_i$ and $\mathbf{r}_i$ replaced by $\mathbf{p}_i'$ and $\mathbf{r}_i'$. Hereafter we shall omit the primes and always refer to the relative motion of the electrons.

An $Al_xGa_{1-x}As$-GaAs-$Al_xGa_{1-x}As$ multilayer structure can be described approximately by such a periodically arranged quantum-well model, in which the mobile carriers are electrons released from donors located in the heavily doped $Al_xGa_{1-x}As$ parts and are essentially confined in the GaAs well regions which are formed by the band discontinuity of $Al_xGa_{1-x}As$-GaAs interfaces. We assume that (i) the potential-well depth is deep enough and tunneling is small enough, so that electrons are confined to just one well, and (ii) the width of the well is narrow and the electron density is not too high, such that electrons occupy only the lowest subband. This description for a semiconductor superlattice has been widely used in the literature. In the effective-mass approximation the lowest subband wave function of the electron in lth well is taken as

$$\psi_{l\mathbf{k}}(\mathbf{r},z)=e^{i\mathbf{k}\cdot\mathbf{r}}\zeta(z-ld)\quad (l=0,\pm1,\ldots) \tag{5}$$

with

$$\zeta(z)=\begin{cases}\left[\frac{2}{a}\right]^{1/2}\cos\left[\frac{\pi z}{a}\right] & \text{for } -\frac{a}{2}\le z<\frac{a}{2}\ , \\ 0 \text{ elsewhere}\ , \end{cases} \tag{6a}$$

(6b)

and the corresponding energy $\epsilon_{\mathbf{k}}=\hbar^2k^2/2m$ is degenerate with respect to the layer indices. Here, $k\equiv|\mathbf{k}|$. Now the Hamiltonian H_e for relative electrons can be written in second quantized representation as

$$H_e=\sum_{l,\mathbf{k},\sigma}\epsilon_{\mathbf{k}}c^\dagger_{l\mathbf{k}\sigma}c_{l\mathbf{k}\sigma}+\frac{1}{2}\sum_{\substack{l,l'\\ \mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}}V_{ll'}(q)c^\dagger_{l,\mathbf{k}+\mathbf{q},\sigma}c^\dagger_{l',\mathbf{k}-\mathbf{q},\sigma'}c_{l',\mathbf{k}',\sigma'}c_{l,\mathbf{k},\sigma}\ , \tag{7}$$

where $c^\dagger_{l\mathbf{k}\sigma}(c_{l\mathbf{k}\sigma})$ are creation (annihilation) operators for relative electrons with lowest subband wave function $\psi_{l\mathbf{k}}$, and $V_{lm}(q)$ is the corresponding matrix element of the Coulomb potential, which can be written as

$$V_{lm}(q)=\frac{e^2}{2\epsilon_0\kappa q}F_{lm}(q)\ , \tag{8}$$

where κ is the background dielectric constant of the superlattice and $F_{lm}(q)$ is a form factor for the Coulomb interaction of the system. For a GaAs-$Al_xGa_{1-x}As$ superlattice, the difference between the dielectric constants in GaAs and $Al_xGa_{1-x}As$ regions is small enough that the image charge contribution is generally neglected, leading to the simple result

$$\begin{aligned}F_{lm}(q)&=F_{l-m}(q)\\ &=\int dz\int dz' e^{-q|z-z'|}\zeta(z-ld)^2\zeta(z'-md)^2\\ &=e^{-q|l-m|d}[\exp(qa)I(q)^2(1-\delta_{lm})+\delta_{lm}H(q)]\ .\end{aligned} \tag{9}$$

Here, δ_{lm} is the Kronecker delta, and the form factors $I(q)$ and $H(q)$ are determined by the electron wave function within the well [Eq. (6)]. Setting $u=qa$, we have[9]

$$\begin{aligned}I(q)&=\int e^{-qz}\zeta(z)^2dz\\ &=4\pi^2[1-\exp(-u)]/[u(u^2+4\pi^2)]\ ,\end{aligned} \tag{10}$$

$$\begin{aligned}H(q)&=\int e^{-q|z-z'|}\zeta(z)^2\zeta(z')^2dz\,dz'\\ &=3\frac{1-\exp(-u)}{u^2+4\pi^2}+\frac{u}{u^2+4\pi^2}\\ &\quad-\frac{1-\exp(-u)}{(u^2+4\pi^2)^2}(u^2-4\pi^2)\\ &\quad+\frac{2}{u}\left[1-\frac{1-\exp(-u)}{u}\right]\ .\end{aligned} \tag{11}$$

In a GaAs-$Al_xGa_{1-x}As$ system the elastic scatterings are mainly due to charged impurities. These charged impurities give rise to an electron-impurity interaction H_{ei} in the Hamiltonian:

$$H_{ei}=\sum_{\substack{l,\sigma,a\\ \mathbf{k},\mathbf{q}}}\frac{Z_ae^2}{2\epsilon_0\kappa q}F_l(q,z_a)e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{r}_a)}c^\dagger_{l,\mathbf{k}+\mathbf{q},\sigma}c_{l,\mathbf{k},\sigma}\ , \tag{12}$$

where $(\mathbf{r}_a,z_a)$ and Z_a are the location and the charge number of the ath impurity and

$$F_l(q,z_a)=\int e^{-q|z-z_a|}\zeta(z-ld)^2dz\ . \tag{13}$$

Image terms have been neglected in Eq. (13). We consider two kinds of impurities: remote impurities and background impurities. The former are the ionized dopants in $Al_xGa_{1-x}As$ regions, which are located in planar sheets at a distance s from the center of each layer with area density N_r per sheet; the latter are distributed equiprobably within the GaAs well regions with area density N_b per layer. Here we assume that there is the same impurity number density in each remote sheet (or in each layer). Thus, to specify an impurity we can use $a=(m,\alpha)$, which denotes the αth impurity in the mth sheet (or mth layer). Its transverse coordinate is $\mathbf{r}_a=\mathbf{r}_{m\alpha}$ and longitudinal position is (for remote impurities)

$$z_a = md - s \quad \left[m = 0, \pm 1, \ldots \text{ and } \frac{a}{2} < s < d - \frac{a}{2} \right], \tag{14}$$

or (for background impurities)

$$z_a = md + z_\alpha \quad \left[m = 0, \pm 1, \ldots \text{ and } -\frac{a}{2} < z_\alpha < \frac{a}{2} \right]. \tag{15}$$

Therefore, for remote impurities

$$F_l(q,z_a) = F(q,l-m,z_\alpha) = \int e^{-q\,|\,z-z_\alpha+(l-m)d\,|}\zeta(z)^2 dz = \begin{cases} F(q,z_\alpha) & \text{if } l=m\ , \\ \exp[-q\,|\,(l-m)d\,|\,]\exp(qz_\alpha)I(q) & \text{if } l>m\ , \\ \exp[-q\,|\,(l-m)d\,|\,]\exp(-qz_\alpha)I(-q) & \text{if } l<m\ , \end{cases} \tag{17}$$

in which ($u \equiv qa$)

$$F(q,z_\alpha) = \frac{8\pi^2}{u(u^2+4\pi^2)}\left[1+\frac{u^2}{2\pi^2}\cos^2\left[\frac{\pi}{a}z_\alpha\right] - 2\exp\left[-\frac{a}{2}\right]\cosh(qz_\alpha)\right]. \tag{18}$$

The phonons in the $Al_xGa_{1-x}As$-GaAs superlattice can be considered approximately the same as in bulk GaAs. They give rise to a phonon part

$$H_{\rm ph} = \sum_{\mathbf{Q},\lambda} \hbar\Omega_{\mathbf{Q}\lambda} b^\dagger_{\mathbf{Q}\lambda} b_{\mathbf{Q}\lambda} \tag{19}$$

and an electron-phonon interaction

$$H_{e\text{-}p} = \sum_{\mathbf{q},q_z,\lambda} M(\mathbf{q},q_z,\lambda) I(iq_z) e^{i\mathbf{q}\cdot\mathbf{R}} (b_{\mathbf{Q}\lambda} + b^\dagger_{-\mathbf{Q}\lambda}) \times \sum_{l,\mathbf{k},\sigma} c^\dagger_{l,\mathbf{k}+\mathbf{q},\sigma} c_{l,\mathbf{k},\sigma}\ , \tag{20}$$

in the Hamiltonian. In these two equations, $b^\dagger_{\mathbf{Q}\lambda}$ ($b_{\mathbf{Q}\lambda}$) are creation (annihilation) operators for the phonons of wave vector $\mathbf{Q}$ in branch λ and frequency $\Omega_{\mathbf{Q}\lambda}$. Here,

$$F_l(q,z_a) = F(q,l-m,-s) = \int e^{-q\,|\,z+(l-m)d+s\,|}\zeta(z)^2 dz = \begin{cases} \exp[-q\,|\,(l-m)d+s\,|\,]I(q) & \text{if } l-m\geq 0\ , \\ \exp[-q\,|\,(l-m)d+s\,|\,]I(-q) & \text{if } l-m<0\ , \end{cases} \tag{16}$$

and for background impurities

$\mathbf{Q} = (\mathbf{q},q_z)$ is the 3D wave vector. In Eq. (20), $M(\mathbf{q},q_z,\lambda) \equiv M(\mathbf{Q},\lambda)$ is the matrix element of the electron-phonon interaction in 3D plane-wave representation and $I(iq_z)$ is a form factor:

$$|\,I(iq_z)\,|^2 = \pi^4 \sin^2 y/[y^2(y^2-\pi^2)^2]\ , \tag{21}$$

with $y \equiv q_z a/2$.

III. FORCE- AND ENERGY-BALANCE EQUATIONS

The derivation of the force- and energy-balance equations in steady-state transport devolves upon the evaluation of the statistical expectation values of the time derivative of the center-of-mass momentum $\dot{\mathbf{P}} = -i[\mathbf{P},H]/\hbar$ and the rate of change of the total relative-electron energy $\dot{H}_e = -i[H_e,H]/\hbar$, or that of the total phonon energy $\dot{H}_{\rm ph} = -i[H_{\rm ph},H]/\hbar$. The procedure is similar to that described in Ref. 5 and will not be repeated here. However, we shall discuss the aspects specifically related to the case of a superlattice.

In steady state, when the center of mass moves at a constant velocity $\mathbf{v}$, the frictional force due to phonons can be shown to be

$$\mathbf{F}_p = 2\sum_{\mathbf{q},q_z,\lambda} |\,M(\mathbf{q},q_z,\lambda)\,|^2\,|\,I(iq_z)\,|^2 \mathbf{q} \sum_{l,l'} e^{-iq_z(l-l')d}\,\hat{\Pi}_2(l,l',\mathbf{q},\Omega_{\mathbf{Q}\lambda}+\mathbf{q}\cdot\mathbf{v})\left[n\left[\frac{\hbar\Omega_{\mathbf{Q}\lambda}}{k_BT}\right] - n\left[\frac{\hbar(\Omega_{\mathbf{Q}\lambda}+\mathbf{q}\cdot\mathbf{v})}{k_BT_e}\right]\right]. \tag{22}$$

Here, T and T_e are the lattice and electron temperatures,[5] respectively; $n(x) \equiv 1/[\exp(x)-1]$ is the Bose function; $\mathbf{v}$ is the center-of-mass velocity or the average drift velocity of the system. $\hat{\Pi}_2(l,l',\mathbf{q},\omega)$ is the imaginary part of the Fourier transform of the electron density-density correlation function of the superlattice $\Pi_2(l,l',\mathbf{q},t)$ defined by

$$\hat{\Pi}(l,l',\mathbf{q},t) = -\frac{i}{\hbar}\theta(t)\sum_{\mathbf{k},\mathbf{k}',\sigma} \langle [c^\dagger_{l,\mathbf{k}+\mathbf{q},\sigma}(t)c_{l,\mathbf{k},\sigma}(t), c^\dagger_{l',\mathbf{k}'-\mathbf{q},\sigma}c_{l',\mathbf{k}',\sigma}] \rangle\ . \tag{23}$$

Here the average is in an equilibrium ensemble of the relative-electron system with Hamiltonian H_e and temperature T_e, imagining it to be decoupled. Also the step function $\theta(t) = 1$ for $t > 0$ and $\theta(t) = 0$ otherwise.

In the absence of Coulomb interaction between carriers, the density-density correlation function has nonzero value only when $l = l'$:

$$\Pi(l,l',\mathbf{q},\omega) = \delta_{ll'}\Pi(\mathbf{q},\omega)\ , \tag{24}$$

and

$$\Pi(\mathbf{q},\omega) = 2\sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}+\mathbf{q}}) - f(\epsilon_{\mathbf{k}})}{\hbar\omega + \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + i\delta} \tag{25}$$

is the density-density correlation function for a single sheet of 2D electrons without Coulomb interaction. $f(\epsilon)=1/\{\exp[(\epsilon-\epsilon_f)/k_BT_e]+1\}$ is the Fermi-Dirac function at temperature T_e and $\epsilon_f=\epsilon_f(T_e)$ is the corresponding temperature-dependent Fermi energy, or chemical potential.

The inclusion of both intralayer and interlayer carrier Coulomb interactions can be achieved using the random-phase approximation (RPA). The well-known RPA treatment leads to the following equation:

$$\hat{\Pi}(l,l',\mathbf{q},\omega)=\delta_{ll'}\Pi(\mathbf{q},\omega)+\Pi(\mathbf{q},\omega)\sum_m V_{lm}(q)\hat{\Pi}(m,l',\mathbf{q},\omega)\ . \tag{26}$$

Assuming an infinite superlattice and neglecting image contributions, we have $V_{lm}(q)=V_{l-m}(q)$ and $\hat{\Pi}(l,l',\mathbf{q},\omega)=\hat{\Pi}(l-l',\mathbf{q},\omega)$ and Eq. (26) reduces to

$$\hat{\Pi}(l,\mathbf{q},\omega)=\Pi(\mathbf{q},\omega)\left[\delta_{l0}+\sum_m V_{l-m}(q)\hat{\Pi}(m,\mathbf{q},\omega)\right]\ . \tag{27}$$

By introducing

$$\hat{\Pi}(q_z,\mathbf{q},\omega)=\sum_l e^{-iq_zld}\hat{\Pi}(l,\mathbf{q},\omega)\ , \tag{28}$$

Eq. (27) is easily solved to give

$$\hat{\Pi}(q_z,\mathbf{q},\omega)=\frac{\Pi(\mathbf{q},\omega)}{1-V(q,q_z)\Pi(\mathbf{q},\omega)} \tag{29}$$

with

$$V(q,q_z)=\sum_l V_l(q)e^{-iq_zld}=\frac{e^2}{2\epsilon_0\kappa q}[H(q)+S(q,q_z)]\ , \tag{30}$$

in which $S(q,q_z)$ comes from the interlayer carrier interaction:

$$S(q,q_z)=\frac{\cos(q_zd)-\exp(-qd)}{\cosh(qd)-\cos(q_zd)}\exp(qa)I(q)^2\ . \tag{31}$$

In terms of the correlation function $\hat{\Pi}(q_z,\mathbf{q},\omega)$, we can rewrite Eq. (22) as a phonon-induced per-layer frictional force $\mathbf{f}_p$:

$$\mathbf{f}_p=2\sum_{\mathbf{q},q_z,\lambda}|M(\mathbf{q},q_z,\lambda)|^2|I(iq_z)|^2\mathbf{q}\hat{\Pi}_2(q_z,\mathbf{q},\Omega_{\mathbf{Q}\lambda}+\mathbf{q}\cdot\mathbf{v})\left[n\left[\frac{\hbar\Omega_{\mathbf{Q}\lambda}}{k_BT}\right]-n\left[\frac{\hbar(\Omega_{\mathbf{Q}\lambda}+\mathbf{q}\cdot\mathbf{v})}{k_BT_e}\right]\right]\ . \tag{32}$$

Note that although $\hat{\Pi}_2(q_z,\mathbf{q},\omega)$ is a periodic function of q_z, $|M|^2|I|^2$ is not. The sum over q_z goes from $-\infty$ to ∞ as usual:

$$\sum_{q_z}\rightarrow(2\pi)^{-1}\int_{-\infty}^{\infty}dq_z\ .$$

The energy loss of the relative-electron system is due to inelastic scattering associated with the electron-phonon coupling. A similar derivation yields the per-layer energy-transfer rate from the electron system to the phonon system:

$$w=2\sum_{\mathbf{q},q_z,\lambda}|M(\mathbf{q},q_z,\lambda)|^2|I(iq_z)|^2\Omega_{\mathbf{Q}\lambda}\hat{\Pi}_2(q_z,\mathbf{q},\Omega_{\mathbf{Q}\lambda}+\mathbf{q}\cdot\mathbf{v})\left[n\left[\frac{\hbar\Omega_{\mathbf{Q}\lambda}}{k_BT}\right]-n\left[\frac{\hbar(\Omega_{\mathbf{Q}\lambda}+\mathbf{q}\cdot\mathbf{v})}{k_BT_e}\right]\right]\ . \tag{33}$$

In deriving the impurity-induced frictional force one needs to average over impurity sites. We assume that there is no interference effect between different kinds of scatterers so that the contributions to the frictional force due to remote- and background-impurity scatterings are additive and the average over these two kinds of impurities can be done separately. Thus we shall evaluate the following quantities:

$$\sum_{m,n}\left\langle\sum_{\alpha,\beta}F(q,l-m,z_\alpha)F(q,l'-n,z_\beta)e^{i\mathbf{q}\cdot\mathbf{r}_\alpha+i\mathbf{q}'\cdot\mathbf{r}_\beta}\right\rangle \tag{34}$$

for background impurities, and

$$\sum_{m,n}\left\langle\sum_{\alpha,\beta}F(q,l-m,-s)F(q,l'-n,-s)e^{i\mathbf{q}\cdot\mathbf{r}_\alpha+i\mathbf{q}'\cdot\mathbf{r}_\beta}\right\rangle \tag{35}$$

for remote impurities. The average is over all the possible configurations of the impurity distribution in the mth and nth layers (sheets). Since $F(q,l-m,z_\alpha)$ is a smooth nonoscillatory function of z_α and the background impurities are distributed equiprobably within each well region, the expression (34) can be simplified approximately as

$$\sum_{m,m'}\overline{F(q,l-m,z)F(q,l'-n,z)}\left\langle\sum_{\alpha,\beta}e^{i\mathbf{q}\cdot\mathbf{r}_\alpha+i\mathbf{q}'\cdot\mathbf{r}_\beta}\right\rangle\ , \tag{36}$$

where

$$\overline{F(q,l-m,z_\alpha)}\equiv\frac{1}{a}\int_{-a/2}^{a/2}F(q,l-m,z)dz=\begin{cases}K(q) & \text{for } l=m\ ,\\ \exp[-q\,|\,(l-m)d\,|\,]\dfrac{\exp(qa)-1}{qa}I(q) & \\ \text{for } l\neq m\ , & \end{cases} \tag{37}$$

with ($u\equiv qa$)

$$K(q)=\frac{8\pi^2}{(4\pi^2+u^2)u}\left[1+\frac{u^2}{4\pi^2}-\frac{1-\exp(-u)}{u}\right]\ . \tag{38}$$

Therefore, in either case, we essentially deal with the quantity

$$A=\left\langle \sum_{\alpha,\beta} e^{i\mathbf{q}\cdot\mathbf{r}_{m\alpha}+i\mathbf{q}'\cdot\mathbf{r}_{n\beta}} \right\rangle . \tag{39}$$

If the impurity distribution is random within each sheet (layer) and there is no correlation between different sheets (layers), the quantity in Eq. (39) is a two-dimensional extension of the averaging discussed by many authors in the 3D case.[10,11] Therefore, to the lowest order of N_I ($N_I=N_r$ or N_b is the impurity sheet density),

$$A=N_I\delta_{\mathbf{q}',-\mathbf{q}} , \tag{40}$$

independent of the layer indices m and n. The assumption of noncorrelation of the impurity distributions in different sheets generally seems reasonable. Nevertheless, as discussed in Ref. 12, the possibility of correlation between the impurity distributions in different layers could be included in the following way. The superlattice system structure enables us to assume that the quantity in Eq. (39) is a function of $m-n$ after configuration averaging:

$$\left\langle \sum_{\alpha,\beta} e^{i\mathbf{q}\cdot\mathbf{r}_{m\alpha}+i\mathbf{q}'\cdot\mathbf{r}_{n\beta}} \right\rangle = N_I\delta_{q',-q}g(m-n) , \tag{41}$$

where the function $g(m)$ ($m=0,\pm1,\ldots$) may be expressed as a Fourier coefficient:

$$g(m)=\frac{d}{2\pi}\int_{-\pi/d}^{\pi/d} dq_z g(q_z)e^{iq_z md} , \tag{42}$$

with the corresponding inverse series

$$g(q_z)=\sum_m g(m)e^{-iq_z md} . \tag{43}$$

The total frictional force due to remote-impurity scattering can now be written as

$$\left[\frac{e^2}{2\epsilon_0\kappa}\right]^2\frac{d}{2\pi}\int_{-d/\pi}^{d/\pi}dq_z\sum_{\mathbf{q}}\frac{\mathbf{q}}{q^2}\sum_{l,l',m,n}F(q,l-m,-s)F(q,l'-n,-s)e^{iq_z(m-n)d}g(q_z)\hat{\Pi}_2(l-l',\mathbf{q},\mathbf{q}\cdot\mathbf{v}) . \tag{44}$$

A similar expression could also be obtained for the background-impurity-induced total force. The summation over the layer indices in Eq. (44) is easy to perform, resulting in the expression for the per-layer frictional force due to remote- and background-impurity scatterings jointly:

$$\mathbf{f}_i=\left[\frac{e^2}{2\epsilon_0\kappa}\right]^2\left[\frac{d}{2\pi}\right]\int_{-d/\pi}^{d/\pi}dq_z\sum_{\mathbf{q}}\frac{\mathbf{q}}{q^2}\tilde{N}(q,q_z)g(q_z)\hat{\Pi}_2(q_z,\mathbf{q},\mathbf{q}\cdot\mathbf{v}) , \tag{45}$$

in which $\tilde{N}(q,q_z)$ is an effective impurity density:

$$\tilde{N}(q,q_z)=N_rZ_r^2\left|\frac{\sinh[q(d-s)]+\exp(iq_zd)\sinh(qs)}{\cosh(qd)-\cos(q_zd)}\right|^2\exp(qa)I(q)^2 + N_bZ_b^2\left[\frac{\cos(q_zd)-\exp(-qd)}{\cosh(qd)-\cos(q_zd)}\frac{\exp(qa)-1}{qa}I(q)+K(q)\right]^2 , \tag{46}$$

and Z_r and Z_b are equivalent charge numbers of the remote and background impurities.

For an uncorrelated distribution of impurities, $g(m)=1$ and $g(q_z)=2\pi\delta(q_zd)$, whence the expression (45) for the impurity-induced per-layer frictional force $\mathbf{f}_i$ reduces to

$$\mathbf{f}_i=\left[\frac{e^2}{2\epsilon_0\kappa}\right]^2\sum_{\mathbf{q}}\frac{\mathbf{q}}{q^2}\tilde{N}(q)\hat{\Pi}_2(0,\mathbf{q},\mathbf{q}\cdot\mathbf{v}) , \tag{47}$$

with

$$\tilde{N}(q)\equiv\tilde{N}(q,0) =N_rZ_r^2\left[\frac{\cosh[q(d/2-s)]}{\sinh(qd/2)}\right]^2\exp(qa)I(q)^2 + N_bZ_b^2\left[\frac{2}{qa}\frac{\exp(qa)-1}{\exp(qd)-1}I(q)+K(q)\right]^2 . \tag{48}$$

Now the force and energy balance equations of steady-state transport can be written down for each layer:

$$N_se\mathbf{E}+\mathbf{f}(\mathbf{v})=0 \tag{49}$$

and

$$\mathbf{v}\cdot\mathbf{f}(\mathbf{v})+w(\mathbf{v})=0 . \tag{50}$$

Here N_s is the carrier area density per layer, and

$$\mathbf{f}(\mathbf{v})=\mathbf{f}_i+\mathbf{f}_p \tag{51}$$

is the per-layer frictional force due to impurity and phonon scatterings, and $w(\mathbf{v})$ is the per-layer energy-loss rate of the electron system.

The carrier mobility, defined by ($v\equiv|\mathbf{v}|$)

$$\mu=v/E , \tag{52}$$

can be written in terms of the per-layer frictional force along the x direction f_x:

$$\frac{1}{\mu}=-\frac{f_x}{eN_sv} . \tag{53}$$

The contributions to $1/\mu$ by different scattering mechanisms (remote and background impurities, acoustic and optical phonons, etc.) are additive within the present lowest-order model, because the frictional forces induced

by different mechanisms are additive. Nevertheless, all these forces depend on the electron temperature, which is to be determined from the energy balance equation involving all the scattering mechanisms jointly.

IV. LINEAR MOBILITY

In the presence of an energy-loss mechanism (electron-phonon interaction), the energy balance equation yields a steady-state solution with electron temperature $T_e = T + O(E^2)$ for weak electric field E. Therefore, the isothermal linear mobility[13] is determined solely by the force balance equation at common electron and lattice temperature T. We have

$$\frac{1}{\mu_{i0}} = -\frac{1}{eN_s}\left[\frac{e^2}{2\epsilon_0\kappa}\right]^2 \sum_{\mathbf{q}} \frac{q_x^2}{q^2}\tilde{N}(q)\frac{\partial}{\partial\omega}\hat{\Pi}_2(0,\mathbf{q},\omega)\,|_{\omega=0} \tag{54}$$

for impurity-limited inverse Ohmic mobility (assume uncorrelated distributions of impurities in different sheets and layers), and [$n'(x) = dn(x)/dx$]

$$\frac{1}{\mu_{L0}} = \frac{2\hbar}{eN_s^2 k_B T}\sum_{\mathbf{q},q_z,\lambda} |M(\mathbf{q},q_z,\lambda)|^2 q_x^2 \hat{\Pi}_2(q_z,\mathbf{q},\Omega_{\mathbf{Q}\lambda}) \times\left[n'\left[\frac{\hbar\Omega_{\mathbf{Q}\lambda}}{k_B T}\right]\right] \tag{55}$$

for phonon-limited inverse Ohmic mobility. These formulas incorporate in full the role of dynamic and temperature-dependent carrier screening represented in the structure of the density-density correlation function of the superlattice [Eq. (23)] within the framework of the RPA.

The remote- and background-impurity-limited Ohmic mobilities have been calculated from Eq. (54) as functions of temperature for several different geometrical parameters of GaAs-$Al_xGa_{1-x}As$ superlattices. [The parameters used in the calculations are GaAs mass density $5.31 g/cm^3$, effective mass $m = 0.07 m_e$ (m_e is the free-electron mass), transverse sound velocity $v_{st} = 2.48\times10^3$ m/s, longitudinal sound velocity $v_{sl} = 5.29\times10^3$ m/s, longitudinal optical-phonon energy $\hbar\Omega_0 = 35.4$ meV, low-frequency dielectric constant $\kappa = 12.9$, optical dielectric constant $\kappa_\infty = 10.8$, acoustic deformation potential $\Xi = 8.5$ eV, and piezoelectric constant $e_{14} = 1.41\times10^9$ V/m.] The results are shown in Fig. 1 (for remote-impurity scattering) and Fig. 2 (for background-impurity scattering), where we plot the inverse Ohmic mobilities μ_{i0}^{-1} normalized by their values at $T = 0$ K, $\mu_{i0}(0)^{-1}$, against temperature from $T = 0.5$ to 400 K, for superlattices with a carrier density $N_s = 2.0\times10^{11}$ cm^{-2} but different well widths a and well separations d. In most cases the inverse Ohmic mobility increases with increasing temperature in the low-temperature region, then decreases after reaching a maximum. This decrease of $1/\mu_{i0}$ at high temperatures is a common feature of impurity-induced linear resistivity when carriers obey Maxwell-Boltzmann statistics. This feature has also been found in both 3D and 2D systems.[5,6,14] Note that the case of $a = 0$ is equivalent to a pure 2D-sheet-array model widely used for a superlattice, in which the electron density has a δ function in the z direction: $|\zeta(z - ld)|^2 = \delta(z - ld)$.

The Ohmic mobilities due to both acoustic and polar optical-phonon scattering have been calculated from Eq. (55) for several different geometrical parameters of

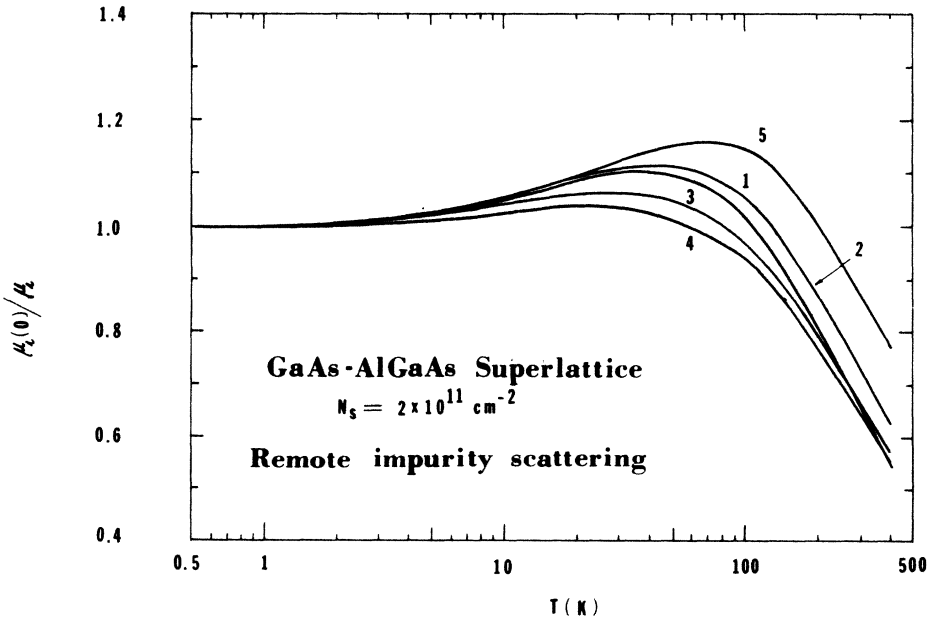

FIG. 1. Normalized inverse Ohmic mobilities $\mu_{i0}(0)/\mu_{i0}$ due to remote-impurity scatterings are shown as functions of temperature for superlattices with carrier density $N_s = 2.0\times10^{11}$ cm^{-2} per sheet but different geometrical parameters (in Å): 1—$a = 0$, $d = 100$, $s = 25$; 2—$a = 0$, $d = 200$, $s = 25$; 3—$a = 50$, $d = 100$, $s = 50$; 4—$a = 100$, $d = 200$, $s = 75$; 5—$a = 200$, $d = 400$, $s = 125$.

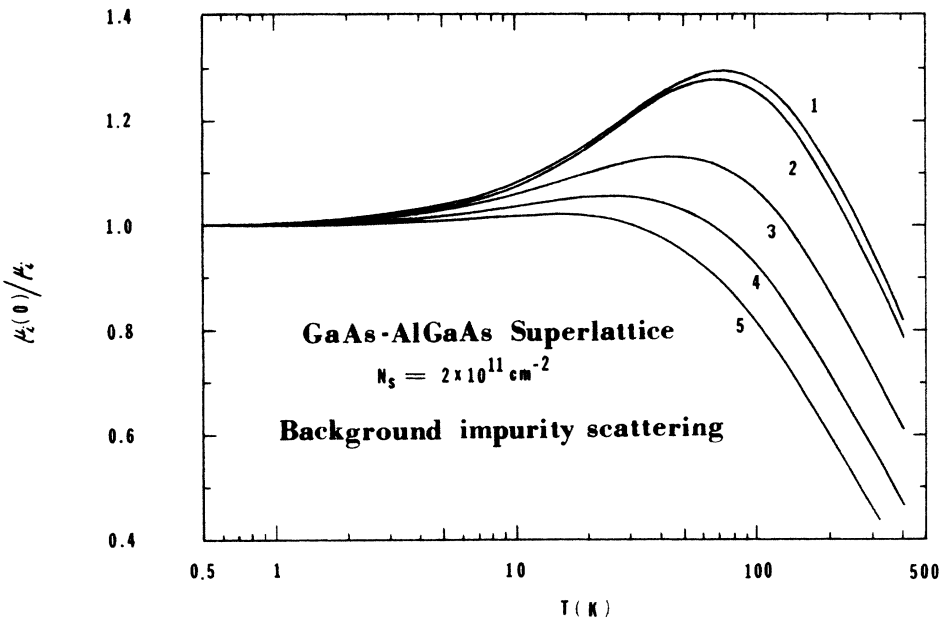

FIG. 2. Normalized inverse Ohmic mobilities $\mu_{i0}(0)/\mu_{i0}$ due to background-impurity scatterings are shown as functions of temperature for superlattices with carrier density $N_s=2.0\times10^{11}$ cm^{-2} per sheet but different geometries (in Å): 1—$a=0$, $d=100$; 2—$a=0$, $d=200$; 3—$a=50$, $d=100$; 4—$a=100$, $d=200$; 5—$a=200$, $d=400$.

GaAs-$Al_xGa_{1-x}As$ superlattices. Acoustic phonons are coupled with electrons via the piezoelectric interaction and deformation potential, and the polar coupling between longitudinal optical phonons and electrons is taken to be the Fröhlich interaction. There are extensive discussions of these electron-phonon interaction mechanisms in the literature.[15–17] The relevant matrix elements pertinent to the present calculation can be found in Ref. 6. In Fig. 3 we plot acoustic-phonon-limited and polar optical-phonon-limited Ohmic mobilities μ_{a0} and μ_{p0} as functions of temperature for four different geometrical parameters of superlattices with the same carrier density $N_s=2.0\times10^{11}$ cm^{-2} per layer. The most striking feature in this figure is the significant difference between curve 1 ($a=0$ Å and $d=100$ Å system) and curve 2 ($a=50$ Å and $d=100$ Å system) for acoustic-phonon-limited mobility at high temperatures ($T>30$ K). This is a clear indication that the 2D-sheet-array model is poor for transport studies where relatively large wave vectors may play a significant role so that the electron confinement should be taken into account. A pure 2D model generally overestimates the electron-phonon scattering.

V. RESULTS FOR NONLINEAR TRANSPORT

Nonlinear steady-state dc transport has been studied numerically from the balance equations (49) and (50) with per-layer frictional forces and energy-transfer rates as given by Eqs. (51), (32), (47) and (33). In this, we take into account both acoustic-phonon scattering (piezoelectric coupling and deformation potential) and polar optical-phonon scattering (Fröhlich interaction). At the same time we consider elastic scatterings due to both remote impurities and background impurities and assume equali-

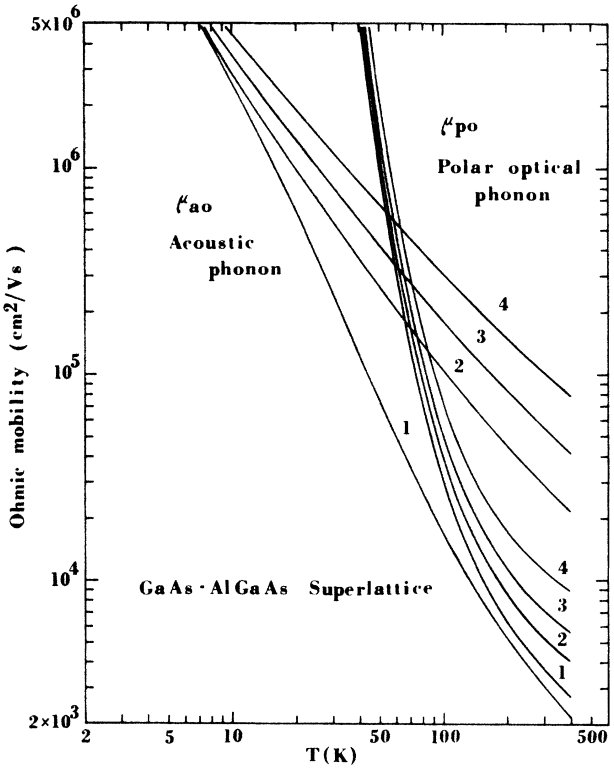

FIG. 3. Ohmic mobilities limited by acoustic-phonon scattering and by polar optical-phonon scattering μ_{a0} and μ_{p0} are shown as functions of temperature for superlattices with carrier density $N_s=2.0\times10^{11}$ cm^{-2} per sheet but different geometrical parameters (in Å): 1—$a=0$, $d=100$; 2—$a=50$, $d=100$; 3—$a=100$, $d=200$; 4—$a=200$, $d=400$.

ty of the contributions of these two kinds of impurities to the Ohmic mobility in the zero-temperature limit. Moreover, the RPA expression [Eq. (29)] for the density-density correlation function of a superlattice is used in the calculation, thereby including full carrier screening and high-field descreening effects as well as plasmon contributions.

The calculated results for the nonlinear mobility μ [defined by Eq. (52)] normalized to its Ohmic limit μ_0, and the electron temperature T_e, are shown as functions of drift velocity v in Figs. 4(a)—4(c) at lattice temperature $T=0$ K for GaAs-$Al_xGa_{1-x}As$ superlattices with carrier density $N_s=2.0\times10^{11}$ cm^{-2} per layer, but different superlattice geometrical parameters (a, d and s), and different zero-temperature Ohmic mobilities μ_0 corresponding to differing effective impurity densities. The nonlinear mobility generally decreases monotonically with increasing drift velocity v. This is usually a feature of systems composed of one kind (same effective mass) of carrier. On the other hand, the electron temperature is not necessarily monotonic in v, as can be seen in Figs. 4(a)—4(c), where the curves labeled 1 (0 K Ohmic mobility $\mu_0=2.5\times10^5$ cm^2/V s) dip as v increases (around $v=2-3\times10^7$ cm/s), reflecting a trend toward an electron-cooling-type phenomenon. Electron cooling arises from a rapid increase of the electron-energy-loss rate with increasing drift velocity at that range of v for which the impurity scattering in the sample is relatively weak compared to electron-phonon scattering. Cooling may occur due to acoustic-phonon coupling at around the sound velocity only in very pure samples.[18] In the present case, however, the decrease of T_e with increasing v is due to polar optical-phonon scattering; it may give rise to a much larger electron-energy-loss rate at large v, resulting in the occurrence of the cooling-type effect in experimentally accessible systems. For given carrier sheet density N_s and Ohmic mobility μ_0 and at fixed drift velocity, the carriers generally stay cooler and show a stronger cooling trend in samples with smaller well width a. This may be attributed to the enhancement of the effective electron-phonon interaction in very thin quantum-well systems. These cooling-type effects may be detected, provided that the electron temperature can be properly determined experimentally. It should be noted that the electron temperature here is not a parameter in a preassumed distribution function for the carriers in transport, but rather it measures the internal energy of the relative-electron system and should thus reflect the strength of the carrier thermal motion. It seems not unreasonable to conjecture that T_e may be estimated from thermal noise measurements on the system.

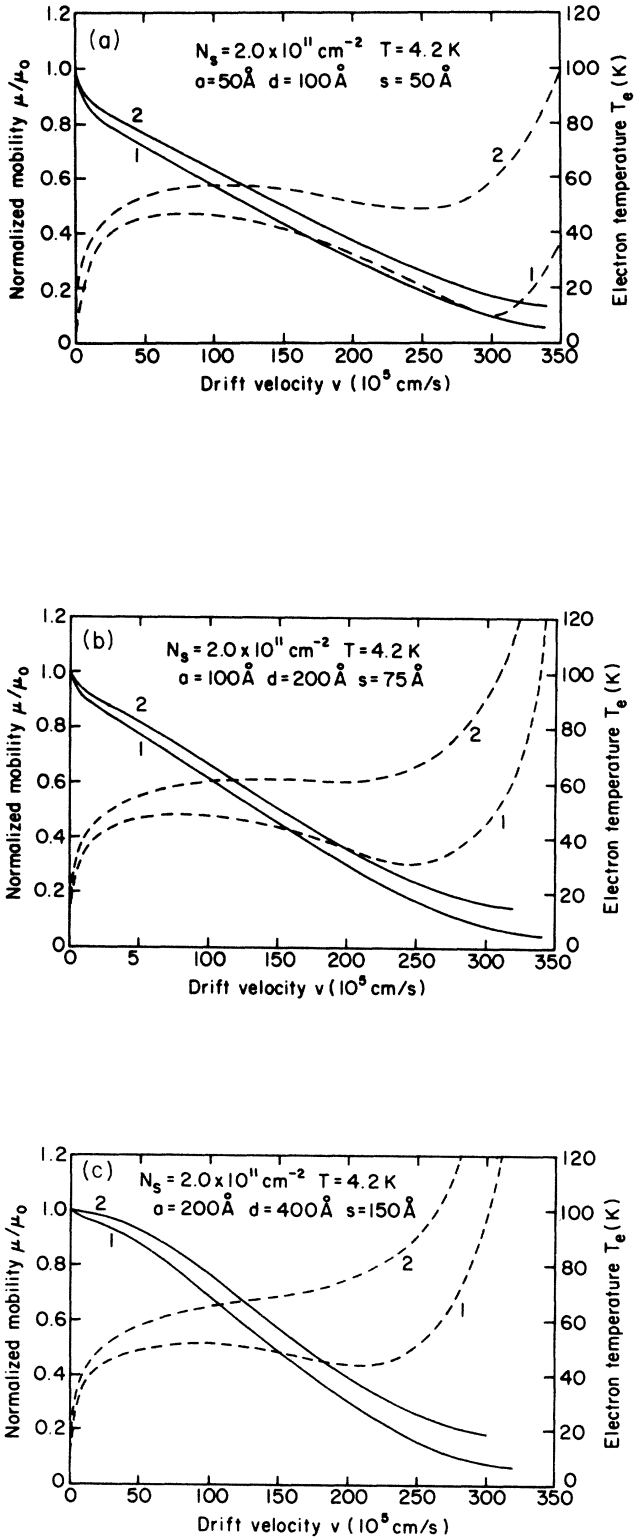

FIG. 4. (a)—(c) Nonlinear mobilities normalized to the Ohmic limit μ/μ_0 (solid curves) and electron temperatures T_e (dashed curves) are shown as functions of drift velocity v at lattice temperature $T=4.2$ K for GaAs-$Al_xGa_{1-x}As$ quantum-well superlattices with carrier density $N_s=2.0\times10^{11}$ cm^{-2} per sheet, but different values of impurity-limited Ohmic mobilities: 1—2.5×10^5 cm^2/V s; 2—8.0×10^4 cm^2/V s.

ACKNOWLEDGMENTS

This work was partially supported by the U.S. Army (Electronic Materials Research Division) at the Electronics Technology and Devices Laboratory, Fort Monmouth, NJ.

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