Theory of Negative Differential Conductivity in a Superlattice Miniband

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Bloch electron conductivity perpendicular to the layers of a superlattice (period d) is evaluated using an extension of the balance-equation approach [X.L. Lei and C. S. Ting, Phys. Rev. B **32**, 1112 (1985)] to narrow-band transport. The perpendicular peak drift velocity v_p and the critical field E_c, at which the drift velocity peaks, are analyzed as functions of miniband width. Our theoretical prediction that $E_c d$ increases with decreasing miniband width agrees well with the data of Sibille *et al.* [Phys. Rev. Lett. **64**, 52 (1990)], even for the samples of narrowest miniband width in their experiment.

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Twenty years ago, Esaki and Tsu[1] proposed that a man-made superlattice structure in which electrons move in a periodic potential on a scale of many lattice constants would facilitate the observation of quantum-mechanical properties of Bloch states in a new domain of physical scale. The narrow wave-vector minizones and the narrow energy bands make it possible for electrons to be accelerated with moderate electric fields beyond the inflection point of the curve of energy ε versus crystal momentum $\mathbf{k}$, entering a regime in which $\partial^2\varepsilon/\partial k^2$ is negative, leading to the prospect of a negative differential conductance (NDC). Subsequent observations of NDC in carrier transport perpendicular to the superlattice layers, however, have been due to the formation of highly localized, high-field domains.[2-4] It was not until the past few years that perpendicular carrier motion was clearly demonstrated to occur through a Bloch-type miniband state.[5] Recently Sibille *et al.*,[6,7] performing systematic measurements and analysis on a series of small-period superlattice samples, were able to show that perpendicular NDC was observed with certainty, and that Bloch electron conduction through the superlattice miniband is responsible for this negative differential mobility over a large range of superlattice parameters. They were able to extract the peak drift velocity v_p and the critical field E_c (at which the drift velocity peaks) in the velocity-field (v-E) curve by analyzing the experimental data. While their results definitively exclude the hopping transport mechanism between Wannier-Stark quantized levels,[8,9] in favor of Bloch miniband transport, the behaviors of v_p and E_c which they observed as functions of miniband width are only in very crude agreement with the theory of Esaki and Tsu.[1]

There have been several Monte Carlo calculations[10-12] on superlattice miniband transport since the pioneering work of Esaki and Tsu. However, a detailed theoretical investigation, even a numerical one, which facilitates direct comparison with experiments, is still lacking. There remains an urgent need to establish a more sophisticated theory, preferably an analytical one, to provide a readily accessible and detailed evaluation of the perpendicular Bloch transport of carriers in a superlattice. In this Letter we report a convenient and succinct calculation based on a balance-equation theory[13] extended[14] to the case of Bloch transport carriers in a superlattice miniband. The idea of this approach is to treat the transporting carriers as a many-particle system and focus on the motion of its center of mass, in contradistinction to methods dealing with individual particle dynamics. We assume that the conducting carriers of the superlattice are free to move in layers (x-y plane), but are subject to a periodic potential in the z direction, with the single-electron state described by a wave vector $\mathbf{k}=(\mathbf{k}_\parallel,k_z)$, $-\pi/d<k_z\le\pi/d$, d being the period of the superlattice, and the wave function written as $\sim\exp(i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel)\phi_{k_z}(z)$. We employ tight-binding sums for the envelope function $\phi_{k_z}(z)$ and $\varepsilon(\mathbf{k})=k_\parallel^2/2m+\varepsilon_1(k_z)$ for the energy disperison relation, with

$$\varepsilon_1(k_z)=\tfrac{1}{2}\Delta(1-\cos k_z d)\,, \tag{1}$$

Δ being the miniband width. The system under consideration involves N interacting electrons in this single miniband under the influence of a uniform electric field $\mathbf{E}=E\hat{\mathbf{z}}$, subject to impurity and phonon scatterings. The total Hamiltonian H of the system is the sum of a phonon part $H_{\rm ph}$, electron-phonon and electron-impurity interactions H_{ep},H_{ei}, a uniform electric-field potential $H_E=-e\mathbf{E}\cdot\sum_j\mathbf{r}_j$, and a band-related effective Hamiltonian

$$H_e=\sum_j\varepsilon(\hat{\mathbf{p}}_j)+H_{ee}\,, \tag{2}$$

representing the electrons in the single energy band with the complement of electron-electron interactions H_{ee}. $\hat{\mathbf{p}}_j\equiv-i\nabla_j$ and $\mathbf{r}_j$ are momentum and position operators of the jth electron. It is convenient to introduce the center-of-mass position and momentum operators

defined as $\mathbf{R}=N^{-1}\sum_j \mathbf{r}_j$ and $\hat{\mathbf{P}}=\sum_j \hat{\mathbf{p}}_j$, and the relative electron position and momentum operators $\mathbf{r}_j'=\mathbf{r}_j-\mathbf{R}$, $\hat{\mathbf{p}}_j'=\hat{\mathbf{p}}_j-\hat{\mathbf{P}}/N$. Our theoretical approach involves the determination of the statistical averages of the rate of change of the electron energy $\langle \dot{H}_e\rangle=-i\langle[H_e,H]\rangle$ and the rate of change of the center-of-mass velocity $\langle\hat{\mathbf{v}}\rangle=-i\langle[\hat{\mathbf{v}},H]\rangle$, with $\hat{\mathbf{v}}=-i[\mathbf{R},H]$. The statistical averages are taken with respect to the density matrix evolving from an initial state in which the center of mass moves at a constant momentum $\mathbf{P}_d\equiv N\mathbf{p}_d$ and relative electrons are subject to a thermoequilibrium distribution with temperature T_e, which generally differs from the lattice temperature T.

The steady-state effective-force and energy balance equations, obtained from $\langle\hat{\mathbf{v}}\rangle=0$ and $\langle\dot{H}_e\rangle=0$, take the form

$$eE/m_z^*+A_i+A_p=0\,, \tag{3}$$

$$eEv_d-W=0\,, \tag{4}$$

with scattering interactions treated explicitly to lowest order. Further implicit scattering dependence occurs through the roles of v_d and T_e, as discussed in detail in Refs. 13–15, where the correspondence with other approaches to transport theory is elucidated. Here we introduce an ensemble-averaged inverse-effective-mass tensor $\mathcal{K}_{ij}$ $(i,j=x,y,z)$, with $\mathcal{K}_{xx}=\mathcal{K}_{yy}=1/m$, $\mathcal{K}_{i\neq j}=0$, and

$$\frac{1}{m_z^*}=\mathcal{K}_{zz}=\frac{2}{N}\sum_{\mathbf{k}}\frac{d^2\varepsilon_1(k_z)}{dk_z^2}f(\bar{\varepsilon}(\mathbf{k}),T_e) \tag{5}$$

to describe the response of the band electron system to an external field. Furthermore, we identify the average drift velocity of the carrier system as

$$v_d=\frac{2}{N}\sum_{\mathbf{k}}v(k_z)f(\bar{\varepsilon}(\mathbf{k}),T_e)\,, \tag{6}$$

where $v(k_z)=d\varepsilon_1(k_z)/dk_z$ is the velocity function in the z direction. In the above equations,

$$f(\bar{\varepsilon}(\mathbf{k}),T_e)=\{\exp([\bar{\varepsilon}(\mathbf{k})-\mu]/T_e)+1\}^{-1} \tag{7}$$

is the Fermi distribution function at the electron temperature T_e; μ is the chemical potential determined by the condition $N=2\sum_{\mathbf{k}}f(\bar{\varepsilon}(\mathbf{k}),T_e)$, and

$$\bar{\varepsilon}(\mathbf{k})=\varepsilon_{\mathbf{k}_\parallel}+\varepsilon_1(k_z-p_d) \tag{8}$$

is the energy of the relative electron. In the effective-force balance equation (3), A_i is the frictional acceleration due to randomly distributed impurities of density n_I,

$$A_i=\frac{2\pi n_I}{N}\sum_{\mathbf{k},\mathbf{q}}|u(\mathbf{q})|^2|g(q_z)|^2[v(k_z+q_z)-v(k_z)]\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k}))\frac{f(\bar{\varepsilon}(\mathbf{k}),T_e)-f(\bar{\varepsilon}(\mathbf{k}+\mathbf{q}),T_e)}{|\epsilon(\mathbf{q},\bar{\varepsilon}(\mathbf{k})-\bar{\varepsilon}(\mathbf{k}+\mathbf{q}))|^2}\,, \tag{9}$$

and A_p is the frictional acceleration due to phonons,

$$A_p=\frac{4\pi}{N}\sum_{\mathbf{k},\mathbf{q},\lambda}|M(\mathbf{q},\lambda)|^2|g(q_z)|^2[v(k_z+q_z)-v(k_z)]\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})+\Omega_{\mathbf{q},\lambda})$$
$$\times\frac{f(\bar{\varepsilon}(\mathbf{k}),T_e)-f(\bar{\varepsilon}(\mathbf{k}+\mathbf{q}),T_e)}{|\epsilon(\mathbf{q},\bar{\varepsilon}(\mathbf{k})-\bar{\varepsilon}(\mathbf{k}+\mathbf{q}))|^2}\left[n\left(\frac{\Omega_{\mathbf{q},\lambda}}{T}\right)-n\left(\frac{\bar{\varepsilon}(\mathbf{k})-\bar{\varepsilon}(\mathbf{k}+\mathbf{q})}{T_e}\right)\right]. \tag{10}$$

In energy balance equation (4), W is the energy-loss rate per electron from the carrier system to the phonon system,

$$W=\frac{4\pi}{N}\sum_{\mathbf{k},\mathbf{q},\lambda}|M(\mathbf{q},\lambda)|^2|g(q_z)|^2\Omega_{\mathbf{q},\lambda}\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})+\Omega_{\mathbf{q},\lambda})$$
$$\times\frac{f(\bar{\varepsilon}(\mathbf{k}),T_e)-f(\bar{\varepsilon}(\mathbf{k}+\mathbf{q}),T_e)}{|\epsilon(\mathbf{q},\bar{\varepsilon}(\mathbf{k})-\bar{\varepsilon}(\mathbf{k}+\mathbf{q}))|^2}\left[n\left(\frac{\Omega_{\mathbf{q},\lambda}}{T}\right)-n\left(\frac{\bar{\varepsilon}(\mathbf{k})-\bar{\varepsilon}(\mathbf{k}+\mathbf{q})}{T_e}\right)\right]. \tag{11}$$

In the above expressions $u(\mathbf{q})$ represents the impurity potential, $M(\mathbf{q},\lambda)$ is the electron-phonon matrix element for phonons of wave vector $\mathbf{q}$ in branch λ, having frequency $\Omega_{\mathbf{q},\lambda}$, $n(x)=(e^x-1)^{-1}$ is the Bose function, and $\epsilon(\mathbf{q},\omega)$ is the dielectric function of the periodic superlattice for carriers in the lowest subband within the random-phase approximation, evaluated at the electron temperature T_e. $g(q_z)$ is a form factor determined by the wave function of the superlattice miniband. In the extreme tight-binding limit for the envelope function it is simply the form factor of a single quantum well:

$$g(q_z)=(2/d)\int_0^{a/2}dz\,|\phi(z)|^2\cos q_z z\,,$$

$\phi(z)$ being the single-well function and a the well width.

The meaning of Eqs. (3) and (4) is physically clear. Equation (3) bespeaks the balance of the resistive force and the electric force experienced by the center of mass, a particle having charge Ne and variable mass Nm_z^*. Equation (4) indicates that the energy supplied by the electric field is dissipated to the phonon system.

Because of the appearance of the center-of-mass momentum in $\bar{\varepsilon}(\mathbf{k})$ [Eq. (8)], the ensemble-averaged inverse effective mass $1/m_z^*$, the average drift velocity v_d, and the other observable quantities are functions of the electron temperature T_e and the center-of-mass momentum p_d. The effective-force and energy balance equations enable us to determine T_e and p_d and thus all the

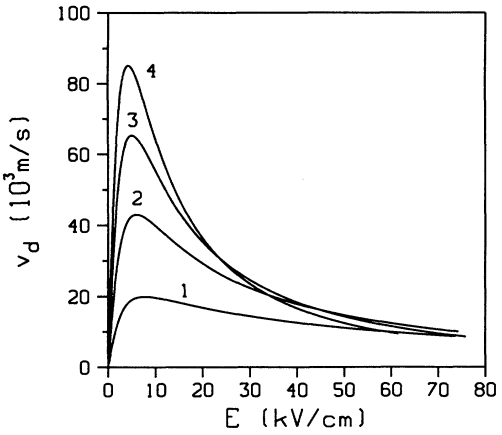

FIG. 1. Calculated drift velocity at lattice temperature $T=300$ K as a function of electric field for a series of GaAs/AlAs superlattices with $N_s=2\times10^{10}$ cm^{-2}, $d=57$ Å, and weak-field mobility $\mu_0=2000$ cm^2/Vs at 4.2 K, having various miniband widths measured in units of temperature as follows: curve 1, $\Delta=300$ K; curve 2, $\Delta=500$ K; curve 3, $\Delta=700$ K; curve 4, $\Delta=900$ K.

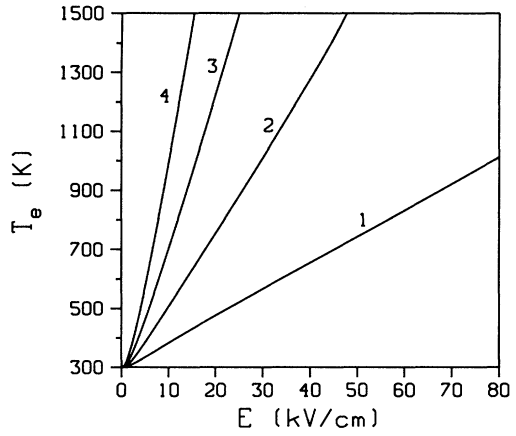

FIG. 2. Electron temperature as a function of electric field for the same series of superlattices as in Fig. 1.

physical quantities for a given electric field E.

The balance equations (3) and (4) have been solved numerically for p_d and T_e as functions of the electric field E at various lattice temperatures T, carrier sheet densities N_s, superlattice periods d, and miniband widths Δ, with parameters pertinent to the Γ-valley electrons in the GaAs/AlAs superlattice of the experiments of Sibille *et al.*[6,7] Scatterings due to impurities, polar-optic phonons, and acoustic phonons (including deformation potential and piezoelectric couplings) are taken into account. Almost all the material parameters are known (such as the electron effective mass, optic-phonon frequency, static and optical dielectric constants, longitudinal and transverse sound velocities, deformation potential, and piezoelectric constant). The only adjustable parameter involved is the impurity scattering rate. A sampling of our results for drift velocity v_d and electron temperature T_e is given, showing their dependences on the electric field, in Figs. 1 and 2 for several miniband widths. In all the cases investigated the velocity-field curve exhibits negative differential mobility with a peak drift velocity v_p at critical field E_c. To compare with the experiments of Sibille *et al.*,[6,7] we plot v_p/d and E_cd as functions of miniband width Δ in Figs. 3(a) and 3(b). The experimental data are taken from the published figures in Ref. 6. Our theoretical curves are calculated assuming that the treated family of superlattices, with differing miniband widths, have the same material parameters and the same impurity scattering rate. The latter is the only parameter which may be adjusted to fit the data. The theoretical curves of the present work are in remarkably good agreement with the experimental data. The only exception is the case of $\Delta\simeq160$ meV,

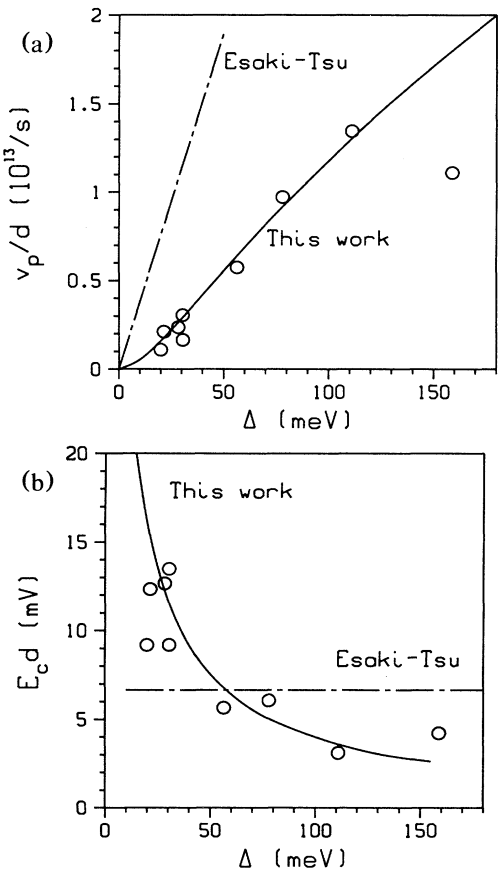

FIG. 3. Dependences of v_p/d and E_cd on the miniband width Δ. Solid curves are calculated using balance equations (3) and (4) at $T=300$ K for GaAs/AlAs superlattices with electron sheet density $N_s=2\times10^{10}$ cm^{-2} and a fixed impurity scattering rate. Experimental data (open circles) are taken from Sibille *et al.* (Ref. 6). Values of v_p/d and E_cd based on Esaki-Tsu theory (with $\tau=0.1$ ps) are also shown (as dot-dashed lines).

which exhibits a lower v_p/d and a higher $E_c d$. This was interpreted by Sibille *et al.* as the onset of the Γ-X Gunn transfer.[6] Another possibility is that this superlattice has stronger impurity scattering. The present theory predicts an increase in $E_c d$ with decreasing Δ for the first time, in favorable comparison with the experimental observations.[6] This strongly supports the conclusion of Sibille *et al.* that miniband Bloch transport is responsible for the observed NDC. Even for the samples investigated having smallest miniband width,[6] Wannier-Stark quantization does not appear necessary to interpret the experimental data. For comparison, we have also included the Esaki-Tsu predictions[1] [$v_p/d = 0.25\Delta/\hbar$ and $E_c d = \hbar/e\tau$, for a sinusoidal $\varepsilon_1(k_z)$; τ is the scattering time] in Figs. 3(a) and 3(b). The nonlinear balance-equation transport dynamics employed here seem to provide an adequate basis for a refined theoretical resolution of the modern classic problem of superlattice miniband transport featuring negative differential conductivity as envisioned by Esaki and Tsu.

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