RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 48, NUMBER 12 15 SEPTEMBER 1993-II

Effect of elastic scattering on miniband transport in semiconductor superlattices

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(Received 22 June 1993)

Within the quasiclassical Boltzmann-Bloch approach to nonlinear miniband transport in superlattices, elastic scattering is included in a relaxation-time approximation. Elastic scattering makes the problem truly three dimensional and leads in the regime of negative differential conductance to results that are qualitatively different from those of the quasi-one-dimensional models considered previously and compare favorably with recent experiments and balance-equation calculations.

Quasiclassical dynamics of Bloch electrons predicts fascinating phenomena such as Bloch oscillations and regimes with negative differential conductivity (NDC), if the electrons can be forced by an applied electric field to follow the periodic band structure through a considerable region in $\mathbf{k}$ space before being scattered. Whereas large Brillouin zones and wide energy bands prohibit these phenomena in natural bulk crystals, Esaki and Tsu[1] predicted a long time ago that they should become observable in semiconductors with artificial superlattices of sufficiently large lattice constants a. Such superlattices create narrow minibands and small Brillouin zones with boundaries which can easily be reached by an electron accelerated by a moderate electric field before it is scattered into another part of the Brillouin zone. The prediction was that the drift velocity v_D of electrons responding to an electric field F applied in the growth (z) direction of the superlattice will decrease with increasing F, once F becomes larger than a critical value $F_{\rm max} = \hbar\nu/ea$, at which the scattering rate ν equals the Bloch-oscillation frequency $eaF/\hbar$. Here $-e$ is the electron charge. In ideal superlattices, the motion in z direction decouples from the lateral motion in the x-y plane, and the calculation of v_D becomes a one-dimensional (1D) problem. Scattering, however, and notably elastic scattering, couples the motion in z direction to the lateral motion, and the problem becomes manifestly three dimensional (3D). The aim of this paper is to emphasize the importance and to discuss the consequences of this coupling of vertical and lateral degrees of freedom, which apparently has not been appreciated before. Previous generalizations of the Esaki-Tsu prediction to finite temperatures using the Boltzmann-Bloch equation in relaxation time approximation are 1D theories in this sense.[2,3] Monte Carlo calculations of the drift velocity[4,5] also did not appreciate the particular 3D nature of scattering, and essentially confirmed the Esaki-Tsu prediction, long before it could be verified experimentally.

So far only two groups have claimed that their experiments reveal the Esaki-Tsu mechanism of miniband transport, and not hopping of electrons between localized states in adjacent wells of the superlattice. Sibille *et al.*[6] systematically studied stationary transport in several superlattices with different miniband widths (Δ) and periods. They reported qualitative agreement with the Esaki-Tsu predictions; however, their $F_{\rm max}$ values seemed to decrease systematically with increasing Δ. The first direct observation of a v_D-F characteristic corresponding to NDC up to F values far beyond the maximum, has been achieved in time-of-flight experiments by Grahn *et al.*[7] They found a good agreement with the finite temperature prediction of the 1D theory,[2,3] at least for higher temperatures, $k_BT > \Delta$.

These experiments, especially the unexpected Δ dependence of $F_{\rm max}$, stimulated a renewed theoretical interest in the problem.[8–10] Lei, Horing, and Cui[8] applied a balance-equation approach[11] to the superlattice model and reported an impressive agreement with the experimental results of Ref. 6. Similar to the Monte Carlo calculations,[4,5] their calculation included explicitly the interaction of the electrons with acoustical and optical phonons as well as with randomly distributed impurities, and, in addition, the screening of these interactions. Although the ansatz of Ref. 8 is very general, it lacks transparency and does not clarify which particular interaction mechanism is responsible for the qualitative differences from the predictions of the 1D Boltzmann-Bloch theories, notably for the Δ dependence of $F_{\rm max}$.

The purpose of this paper is to discuss a transparent theory of the NDC in miniband transport with a minimum of assumptions and model parameters, in order to gain a deeper physical understanding of the apparent insufficiencies of the 1D theories. The basic idea is that elastic scattering by impurities or interface roughness will transfer energy, gained by the electron during its motion in the field direction, to the lateral degrees of freedom. Thus, elastic scattering will effectively render the problem a really three-dimensional one, and should be treated explicitly. In order to do this in the most simple and transparent way, we describe it, in addition to inelastic scattering, by a simple relaxation rate in a Boltzmann-Bloch equation.

As in previous work,[1–5,8–10] we take the tight-binding energy

$$E_1(k_z) = \tfrac{1}{2}\Delta(1 - \cos ak_z) \qquad (1)$$

in the z direction and free motion with effective mass m in the lateral directions,

$$E(\mathbf{k}) = \hbar^2 k_\perp^2/2m + E_1(k_z)\,, \qquad (2)$$

with $k_\perp^2 = k_x^2 + k_y^2$.

The stationary Boltzmann-Bloch equation is written as

$$-\frac{eF}{\hbar}\frac{\partial}{\partial k_z} f(\mathbf{k}) = -\nu_{\rm in}\left\{f(\mathbf{k}) - f_0[E(\mathbf{k})]\right\} + C_{\rm el}(f,\mathbf{k})\,, \tag{3}$$

where the inelastic scattering rate $\nu_{\rm in}$ describes relaxation towards the equilibrium distribution function f_0. If elastic scattering is neglected, $C_{\rm el} = 0$, and if nondegenerate statistics is assumed, one obtains the well-known result for the drift velocity,[2,3]

$$v_D = v_0\,\{(F/F_0)/[1 + (F/F_0)^2]\}\; Q\,(k_B T/\Delta)\,, \tag{4}$$

where $v_0 = -a\Delta/2\hbar$, and $Q(t) = I_1(1/2t)/I_0(1/2t)$ with modified Bessel functions I_ν. The maximum of v_D occurs at the electric field $F_0 = \hbar\nu_{\rm in}/ae$. The original Esaki-Tsu result follows in the limit $T \to 0$, with $Q(0) = 1$.

In order to simulate elastic scattering, we introduce in the Boltzmann equation (3) the collision term

$$C_{\rm el}(f,\mathbf{k}) = -\nu_{\rm el}\,\{\,f(\mathbf{k}) - \Phi_f[E(\mathbf{k})]\,\}\,. \tag{5}$$

Here

$$\Phi_f(E) = \alpha\int d^3k'\;\delta\,[E - E(\mathbf{k}')]\;f(\mathbf{k}')\,/\,D(E) \tag{6}$$

is the average of the distribution function taken over surfaces of constant energy, $E(\mathbf{k}') = E$, $D(E)$ is the density of states, and $\alpha = 2/(2\pi)^3$. This ansatz describes back and forth scattering with equal weights between the state $\mathbf{k}$ and all states $\mathbf{k}'$ of the same energy. It effectively couples the motion in superlattice direction to the lateral degrees of freedom. Before proceeding, we stress that our 3D model is qualitatively different from the corresponding 1D model discussed by Ignatov, Dodin, and Shashkin[9] (IDS). The IDS model couples the motion in the z direction only to that in the $-z$ direction, but not to the lateral degrees of freedom. As a consequence, the drift velocity can be calculated analytically. The result can be written in the form of Eq. (4), if one replaces v_0 with $v_0^{\rm IDS} = v_0\delta^{1/2}$ and F_0 with $F_0^{\rm IDS} = \delta^{1/2}\hbar\nu_{\rm tot}/ea$, where $\nu_{\rm tot} = \nu_{\rm in} + \nu_{\rm el}$ is the total scattering rate and $\delta = 1 - (\nu_{\rm el}/\nu_{\rm tot})$. This model yields a suppression of the drift velocity below the value of Eq. (4). It cannot, however, explain a Δ dependence of $F_{\rm max}$. Moreover, it predicts the same temperature dependence of the drift velocity as Eq. (4), namely, a simple scaling factor which does not change the shape of the v_D-F curve.

For our 3D model, the drift velocity cannot be calculated analytically. With the dimensionless quantities $\varepsilon = E/\Delta$ and $\xi = F/F_0$ where $F_0 = \hbar\nu_{\rm tot}/ea$, our Boltzmann equation has the formal solution

$$f(k_\perp,k_z) = \frac{a}{\xi}\,e^{ak_z/\xi}\int_{k_z}^{\infty} dk_z'\,e^{-ak_z'/\xi}\,g_f[\varepsilon(k_\perp,k_z')], \tag{7}$$

where

$$g_f(\varepsilon) = (1 - r_e)\,f_0(\varepsilon) + r_e\,\Phi_f(\varepsilon\Delta) \tag{8}$$

and $r_e = \nu_{\rm el}/\nu_{\rm tot}$. Inserting (7) into the definition (6), we obtain an integral equation for g_f which can be written in the form

$$g_f(\varepsilon) - (1 - r_e)\,f_0(\varepsilon) = \frac{r_e}{z(\varepsilon)}\int_{-z(\varepsilon)}^{z(\varepsilon)} dz\int_0^{\infty} du\,e^{-2u}\,g_f\left[\varepsilon - \sin^2 z + \sin^2(z + \xi u)\right]\,. \tag{9}$$

Here, we have inserted the density of states, $D(E) = (2m/\pi^2 a\hbar^2)\,z(E/\Delta)$, with $z(\varepsilon) = \arcsin(\sqrt{\varepsilon})$ if $0 < \varepsilon \le 1$, and $z(\varepsilon) = \pi/2$ if $\varepsilon \ge 1$. In view of the low electron densities in the experiments,[6,7] we present numerical results only for nondegenerate statistics, $f_0(\varepsilon) = \exp(-\varepsilon/t)$, where $t = k_B T/\Delta$ is the reduced temperature. Figure 1 shows Φ_f for different situations. As compared with the equilibrium case ($\xi = 0$), in a stationary state with applied field ($\xi > 0$) electrons are redistributed from states with lower energy to states with higher energy. This "heating" of the electron system is even increased, if part of the scattering is elastic. Apparently, this heating cannot be described by the equilibrium distribution at an elevated electron temperature $T_e > T$, since this would lead to a straight line in Fig. 1, because $\Phi_f = f$ if f depends on $\mathbf{k}$ only via the energy. The cusp behavior at $\varepsilon = 1$ is, of course, closely related to the van Hove singularity of the density of states.

The drift velocity is defined by

$$v_D = \alpha\int d^3k\,v_z(k_z)\,f(\mathbf{k})\,/\,n_e\,, \tag{10}$$

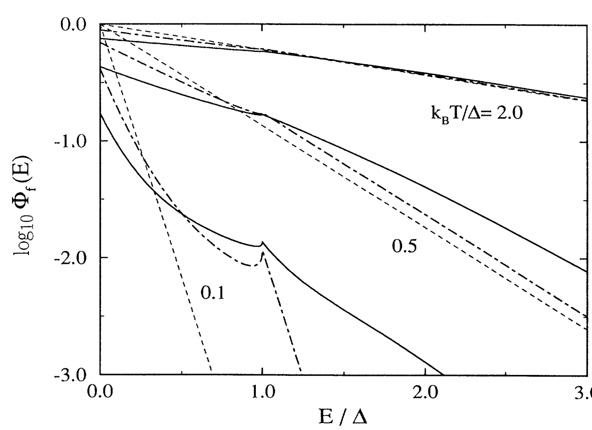

FIG. 1. Average of the distribution function over surfaces of constant energy, as defined in Eq. (6), vs energy for three values of the reduced temperature and, in each case, for thermal equilibrium $f_0(\varepsilon)$=exp$(-E/k_BT)$ (F=0, thin broken lines), for a stationary state with purely inelastic scattering (F=F_0, r_e=0, dash-dotted lines), and for the stationary state with partly elastic scattering (F=F_0, r_e=0.75).

with $v_z(k_z) = \hbar^{-1} dE_1/dk_z$. The normalization constant is the electron density,

$$n_e = \alpha \int d^3k\, f(\mathbf{k}) = \int_0^\infty dE\, D(E)\, \Phi_f(E)\,. \qquad (11)$$

Since n_e in the stationary state has the same value as in the equilibrium state without applied electric field, we may replace in Eq. (11) Φ_f with f_0. We used this sum rule for Φ_f to check our numerical results. With the formal solution (7) the integral in Eq. (10) can be evaluated to yield v_D again in the form of Eq. (4), but now with

$$Q(r_e, \xi, t) = \int_0^1 d\varepsilon\, g_f(\varepsilon) \sqrt{\varepsilon(1-\varepsilon)} \Big/ \int_0^\infty d\varepsilon\, z(\varepsilon)\, f_0(\varepsilon)\ . \qquad (12)$$

In the absence of elastic scattering, $r_e = 0$, one has $g_f = f_0$, and Q is independent of ξ. With $f_0(\varepsilon) = \exp(-\varepsilon/t)$ one exactly recovers Eq. (4). For degenerate statistics this factor $Q(t)$ is, of course, different. For $r_e > 0$, Q depends via ξ on the electric field. Then the shape of the v_D-F curves is different from the Esaki-Tsu result and changes with changing temperature. Two limits can easily be discussed analytically. The first is the linear response regime, $\xi \ll 1$. Here one obtains from Eq. (9) $g_f = f_0 + O(\xi^2)$. Thus, up to first order in ξ, the distribution function and the drift velocity depend only on the total scattering rate, and $Q(0,0,t)$ is a sufficient approximation. A distinction between elastic and inelastic scattering is irrelevant in the linear response regime. The other trivial limit is that of extremely high temperatures, where $f_0(\varepsilon)$ becomes a constant independent of ε. In this limit the solution of Eq. (9) is the constant $g_f = f_0$, and again $Q(0,0,t)$ is sufficient. Thus, our result should approach the 1D form (4) in the linear response regime and, for arbitrary values of ξ, in the limit of high temperatures, provided we define the scaling field as $F_0 = \hbar\nu_{\rm tot}/ea$.

In Fig. 2 we present typical results of our numerical calculations for three values of the temperature and for three values of the ratio $r_e = \nu_{\rm el}/\nu_{\rm tot}$, keeping $\nu_{\rm tot}$ fixed. For $r_e = 0$ (dashed lines) we get the results of the 1D theories:[1,9] with increasing temperature the curves are reduced by an F-independent factor, but their shape does not change. For fixed reduced temperature and increasing r_e, the shape of the curves changes, the maxima are reduced and shifted to smaller values of F. This behavior is qualitatively similar to, but *quantitatively* different from the results of Ref. 9. For fixed $r_e > 0$, the position of the maximum shifts with increasing temperature to larger values of F, so that the effect of elastic scattering is largest at low temperatures and becomes small at high temperatures. This result is *qualitatively* different from that of the 1D model of Ref. 9. It is, however, in qualitative agreement with that of Ref. 8. Systematic results for the dependence of the position $F_{\rm max}$ and the height $(v_D)_{\rm max}$ of the maxima on the scattering-rate ratio r_e and the reduced temperature k_BT/Δ are presented in Figs. 3 and 4, respectively. The results of the 1D model of Ref. 9 would appear in Fig. 3 as horizontal straight lines at $(F/F_0)_{\rm max} = (1-r_e)^{1/2}$ and in Fig. 4 as curves with the same shape as that for $r_e = 0$ (curve 9), but rescaled by a constant factor $(1-r_e)^{1/2}$.

In conclusion, we have emphasized the fact that elas-

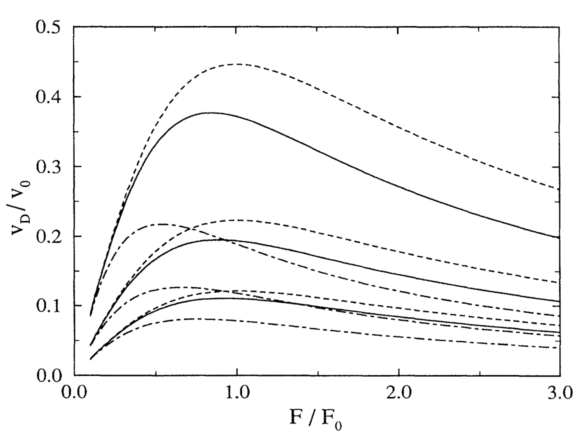

FIG. 2. Calculated drift velocity v_D vs electric field F for r_e= 0.0 (dashed lines), 0.5 (solid lines), and 0.9 (dash-dotted lines), and, in each case, for k_BT/Δ = 0.1, 0.5, and 1.0 (from top to bottom). The units are $v_0 = -a\Delta/2\hbar$ and $F_0 = \hbar\nu_{\rm tot}/ea$, where $\nu_{\rm tot}$ is fixed.

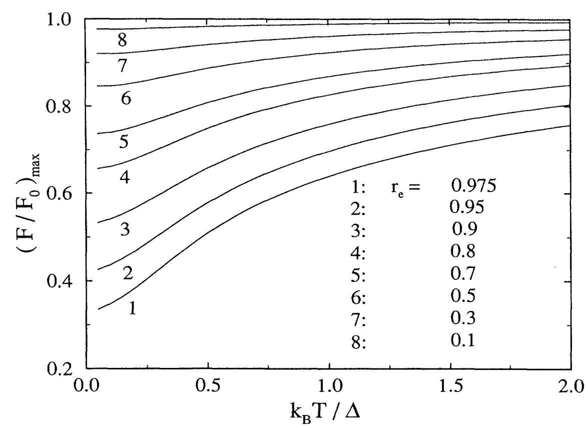

FIG. 3. Electric field values at the maxima of curves as shown in Fig. 2 vs reduced temperature for several values of r_e. Symbols have the same meaning as in Fig. 2.

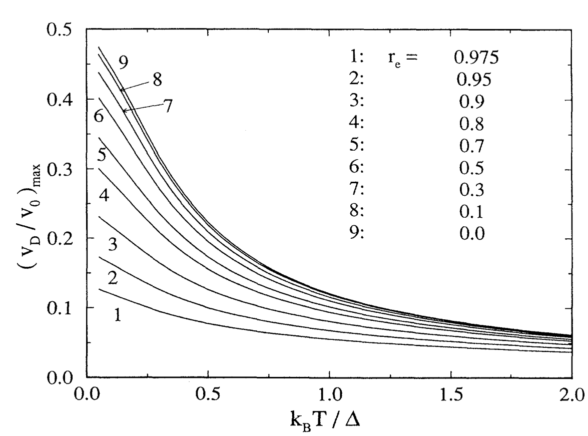

FIG. 4. Maximum values of curves as shown in Fig. 2 vs reduced temperature for different values of r_e.

tic scattering makes the miniband transport through a 1D superlattice in a 3D semiconductor effectively a 3D problem. Incorporating this into a Boltzmann equation in the simple relaxation time approximation, we obtain qualitative deviations from the results of the previously studied 1D theory. Our results are in good qualitative agreement with the very sophisticated calculation of Lei, Horing, and Cui.[8] Quantitative agreement cannot be expected, since our model does not contain any detailed information about scattering matrix elements or screening, and even assumes the scattering rates to be independent of energy. In principle such detailed information could be incorporated into a Boltzmann-Bloch treatment. But this would be at the expense of transparency, and, perhaps more important, these details are not well known for semiconductors with superlattices. For a meaningful comparison with the experimental results of Sibille *et al.*,[6] we would have to assume that, at a given temperature, the scattering rates are the same for superlattices with different miniband widths Δ. Then we conclude, e.g., from Fig. 3 that the electric field $F_{\max}$ at maximum drift velocity should decrease with increasing Δ. This is in agreement with the data of Ref. 6, but these data scatter by about 30%, so that the assumption about the scattering rates becomes questionable. Therefore, we do not attempt a quantitative fit. From a rough estimate, we conclude that in their experiment the elastic scattering rate must be more than an order of magnitude larger than the inelastic one. Considering the experiments of Grahn *et al.*,[7] is seems not surprising that at relatively high temperature good agreement with the result of the 1D theory[3] is obtained, although this indicates that elastic scattering is not so predominant in this situation.

It should be mentioned that, for a known period and bandwidth of the superlattice, the total scattering rate can be evaluated from the linear response regime, i.e., from the low-field mobility, whereas the field $F_{\max}$ at maximum then allows us to extract the ratio of the scattering rates from Fig. 3. This can be done at each value of the lattice temperature T.

Of course, we can also calculate the heating of the electron system within our approach. But since this is not easily accessible to experiments, we postpone this information to a more detailed publication, where we will also discuss the degenerate case, which is not relevant for the experiments mentioned here. We also postpone the similar, though in detail different, case of a lateral superlattice in a 2D electron gas. This situation may become of great interest in the future, since such superlattices can be fabricated with wide and well-isolated minibands and very high mobility,[12] so that pronounced NDC and related effects can be expected to occur already at low applied fields.

Stimulating discussions with Wolfgang Müller and Holger Grahn are gratefully acknowledged. For critical reading of the manuscript I am indebted to V. Fal'ko, D. Pfannkuche, and D. Weiss.

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