Theory of conductivity in superlattice minibands

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We have calculated the impurity-scattering–limited electrical conductivity for vertical transport in superlattice minibands. For sufficiently small carrier density and/or "large" disorder the collisional broadening $\Gamma(\mu)$ can be larger than the chemical potential μ. In such situations the quasiparticle approximation breaks down, and use of the conventional Bloch-Boltzmann transport theory is unreliable. Also, as the period of the superlattice increases, the ratio $\Gamma(\mu)/\mu$ grows, resulting in a reduction of the mobility, leading eventually to Anderson localization. In addition, the carriers in the miniband become nondegenerate already at low temperatures, giving rise to a significant temperature dependence of the mobility. Furthermore, due to the unique shape of the Fermi surface of the superlattice the mobility becomes independent of the carrier density when the chemical potential exceeds the miniband width.

Many interesting transport properties[1] in superlattice minibands, such as Bloch oscillations, are based on the assumption that the Bloch states are well defined. Recently Deveaud *et al.*[2] have firmly established experimentally that electron and hole transport in superlattice minibands is indeed possible through extended Bloch states. The transport along the superlattice axis is important also from a device point of view. Superlattice photoconductors[3] are one example of such an application. Undoubtedly, the investigation of miniband transport is becoming a very active area of research.[4]

Transport in superlattice minibands is unique and interesting since the Fermi energy can be comparable to the single-particle relaxation time and the temperature of the system. This unusual condition is possible because the miniband width falls exponentially with the increasing superlattice period. For example, for holes in the $GaAs/Al_xGa_{1-x}As$ system the bandwidth[2] is only 2.3 meV when the superlattice period is 60 Å. Under these unusual circumstances one must reexamine the quasiparticle approximation used in deriving the conventional Boltzmann equation. We believe that these features make the miniband-transport problem a very interesting fundamental problem.

Another interesting feature is the extreme anisotropy of the superlattice Fermi surface, resulting from the very different motions of a carrier parallel and perpendicular to the superlattice axis (in this paper, we use the expression "parallel" to mean parallel to the superlattice axis). The perpendicular motion is of the free-electron type. However, the parallel motion, which is the subject of this paper, is of the tight-binding type since the carrier moves in the periodic superlattice potential. The density of states can be shown to be flat above a Van Hove singularity, and we will investigate the effect of this on the conductivity.

In this work we include both the relaxation time and the anisotropic effects in the Kubo formula and compute the conductivity without using the quasiparticle approximation. At this stage we are restricting outselves to the linear response region, and neglecting problems associated with localization physics, which becomes important as the miniband width (disorder) decreases (increases). As we show in this paper, there are a number of interesting fundamental questions already in this diffusive miniband-transport region.

There are four relevant scattering mechanisms that may affect miniband transport at low temperatures: (1) intralayer scattering, (2) fluctuations in the layer thickness, (3) compositional fluctuations, and (4) impurities and defects. A first-principles study including all these processes is a difficult task. However, the most important effect of these processes is that Bloch states acquire a finite lifetime. In this paper we restrict ourselves to elastic scattering only, so that this lifetime is a momentum relaxation time. At higher temperatures phonon scattering will become important. Thus, for simplicity, we can model these damping effects by a short-ranged interaction (δ-function impurity scattering). This model has the advantage that one can find a simple analytical expression for the conductivity at zero temperature and, also, the magnitude of the broadening can be incorporated in the theory by a single parameter. This simple model captures some essential features of the system. In our study the interminiband transitions are neglected and we keep a single miniband in our calculations.

The salient features of our results are the following. First, for sufficiently large impurity and/or small carrier densities the quasiparticle approximation breaks down. This is because the damping rate exceeds the chemical potential μ, i.e., $\Gamma(\mu)>\mu$. Thus at these densities the conventional Boltzmann equation is unreliable. It should be emphasized that in superlattice minibands the condition $\Gamma(\mu)>\mu$ does not imply a strong disorder, i.e., $1/(k_F l)>1$, where k_F and l are, respectively, the Fermi wave vector and the mean free path [see Eq. (15)]. Thus quasiparticle approximation of conventional Bloch-Boltzmann transport breaks down in miniband transport before strong localization effects become very important.

Second, the mobility decreases appreciably as $\Gamma(\mu)/\mu$,

the ratio between the imaginary part of the self-energy and the chemical potential, increases. Physically this is because the large damping rate $\Gamma(\mu)$ alters the carrier distribution function significantly around the Fermi surface, and thus the scattering is no longer limited just to the Fermi surface. This reduction of the mobility is consistent with experimental[2] findings of Deveaud *et al.*

Third, the mobility depends significantly on the temperature even in the low-temperature nonphonon regime. Again this is due to the change of the carrier distribution function in the temperature range T around the chemical potential. In superlattice minibands this change is significant since the chemical potential is unusually small, i.e., the carriers become nondegenerate already at low temperatures. This is in sharp contrast to the corresponding three-dimensional situation where the temperature dependence of mobility is small at low temperatures.

Fourth, even when the chemical potential exceeds the miniband width, the current will be nonzero. This is a consequence of the geometrical shape of the Fermi surface with a flat density of states above the Van Hove singularity at the bandwidth.

We now proceed to sketch our theory and calculations. The real (Δ) and imaginary (Γ) parts of the retarded self-energy[5] due to the impurity scattering can be computed in the renormalized Born approximation[6]

$$\Delta(\varepsilon)=\begin{cases}0, & 0<\varepsilon<2W\\ \dfrac{n_i\,|\,c\,|^2 m_\parallel}{2\pi^2\hbar^2}\displaystyle\int_0^{\pi/a}dk_z\ln\left|\frac{\varepsilon-\varepsilon_{k_z}}{\varepsilon_{k_z}}\right|, & \varepsilon>2W\ ,\end{cases} \tag{1}$$

$$\Gamma(\varepsilon)=\begin{cases}0, & \varepsilon<0\\ \dfrac{n_i\,|\,c\,|^2 m_\parallel}{2\pi\hbar^2}\dfrac{1}{a}\cos^{-1}\left[\dfrac{-\varepsilon+W}{W}\right], & 0<\varepsilon<2W\\ \dfrac{n_i\,|\,c\,|^2 m_\parallel}{2\hbar^2 a}, & \varepsilon>2W\ .\end{cases} \tag{2}$$

Here we have taken the impurity scattering to be zero ranged in real space so that it is a constant in momentum space. The constants c, n_i, $m_\parallel$, and a are, respectively, the strength of the renormalized impurity scattering in momentum space, the impurity density, the in-plane effective mass, and the period of the superlattice. In our theory, $\lambda=n_i\,|\,c\,|^2$ is a convenient measure of the strength of disorder in the problem. We parametrize all scattering by this single parameter. In Eqs. (1) and (2), ε and W are, respectively, the carrier energy and half the miniband width.

The energy-momentum dependence in the miniband is taken to be of the simple tight-binding form

$$\varepsilon(\mathbf{k})=\varepsilon_{\mathbf{k}_\parallel}+\varepsilon_{k_z}=\frac{\hbar^2 k_\parallel^2}{2m_\parallel}+W[1-\cos(k_z a)]\ . \tag{3}$$

$2W$ is the bandwidth of the superlattice miniband. We note that both $\Delta(\varepsilon)$ and $\Gamma(\varepsilon)$ develop cusps at the miniband width and this reflects the Van Hove singularity in the density of states at $\varepsilon=2W$;

$$g(\varepsilon)=\begin{cases}\dfrac{m_\parallel}{\pi^2\hbar^2 a}\cos^{-1}\left[\dfrac{-\varepsilon+W}{W}\right], & \varepsilon<2W\\ \dfrac{m_\parallel}{\pi\hbar^2 a}, & \varepsilon>2W\ .\end{cases} \tag{4}$$

In computing the conductivity there is no vertex correction since impurity scattering is isotropic in our model. The conductivity is then given by

$$\sigma=\sigma_1+\sigma_2 \tag{5}$$

where

$$\sigma_1=\hbar e^2\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\left[\frac{-\partial f}{\partial\varepsilon}\right]\int\frac{d^3k}{(2\pi)^3}\frac{A(\mathbf{k},\varepsilon)}{\Gamma(\varepsilon)}\,|\,\mathbf{v}_z(\mathbf{k})\,|^2\ , \tag{6}$$

$$\sigma_2=-2\hbar e^2\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\left[\frac{-\partial f}{\partial\varepsilon}\right]\times\int\frac{d^3k}{(2\pi)^3}[\mathrm{Re}G^2_{\mathrm{ret}}(\mathbf{k},\varepsilon)]\,|\,\mathbf{v}_z(\mathbf{k})\,|^2\ , \tag{7}$$

with

$$G^2_{\mathrm{ret}}(\mathbf{k},\varepsilon)=\frac{1}{[\varepsilon-\varepsilon_{\mathbf{k}}-\Delta(\varepsilon)+i\Gamma(\varepsilon)]^2}\ , \tag{8}$$

and the dressed spectral function is given by

$$A(\mathbf{k},\varepsilon)=\frac{2\Gamma(\varepsilon)}{[\varepsilon-\varepsilon_{\mathbf{k}}-\Delta(\varepsilon)]^2+\Gamma^2(\varepsilon)}\ . \tag{9}$$

The Fermi function and the velocity along the superlattice axis are given by

$$f=\frac{1}{e^{(\varepsilon-\mu)/k_B T}+1}\ , \tag{10}$$

$$\mathbf{v}_z(k)=\frac{1}{\hbar}\frac{\partial\varepsilon_{\mathbf{k}}}{\partial\mathbf{k}_z}. \tag{11}$$

Combining σ_1 and σ_2, we find

$$\sigma=\hbar e^2\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\int\frac{d^3k}{(2\pi)^3}A^2(\mathbf{k},\varepsilon)\,|\,\mathbf{v}_z(\mathbf{k})\,|^2\left[\frac{-\partial f}{\partial\varepsilon}\right]\ . \tag{12}$$

The chemical potential μ is obtained from the particle conservation

$$n=2\sum_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}A(\mathbf{k},\varepsilon)f(\mathbf{k})\ , \tag{13}$$

where n is the density of carriers.

In the limit $\Gamma \to 0$ the second part of the conductivity, σ_2, vanishes, i.e., $\sigma = \sigma_1$, which gives us the usual quasiparticle approximation of the conventional Bloch-Boltzman transport theory. With this quasiparticle approximation,

$$A(\mathbf{k},\varepsilon) = 2\pi\delta(\varepsilon - \varepsilon_{\mathbf{k}} - \Delta(\varepsilon)) , \tag{14}$$

in σ_1 we recover the usual result for the conductivity derived from the Boltzmann equation. However, in superlattice minibands Γ is not always smaller than the chemical potential, and, therefore, it is important to include σ_2 in σ as we do in this paper.

The basic assumption of our theory is the validity of the Bloch picture. Thus, the mean free path l must be larger[3] than the superlattice period $v_z(\mu)\tau(\mu) > a$ or

$$W\left[\frac{v_z(\mu)}{v_{\max}}\right] > \frac{\hbar}{\tau(\mu)} \tag{15}$$

where

$$v_{\max} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k_z}\bigg|_{k_z=\pi/2a} = \frac{Wa}{\hbar} \text{ and } \tau(\mu) = \frac{\hbar}{2\Gamma(\mu)} .$$

For $l < a$, the Bloch-Boltzmann transport picture fails and the Ioffe-Reggel criterion is satisfied, leading to Anderson localization.

Since the general result for the conductivity has to be obtained numerically, it is desirable to have a simple analytical expression. We find, *using the quasiparticle approximation,* that at $T=0$ the conductivity can be written in the Drude form

$$\sigma = \frac{n^* e^2 \tau(\mu)}{m_z} \tag{16}$$

where

$$\tau(\mu) = \frac{\hbar}{2\Gamma(\mu)} , \tag{17}$$

$$n^* = \frac{m_\parallel W}{\hbar^2 a \pi^2}\int_0^{k_F} dk_z \left|\frac{\mathbf{v}_z(\mathbf{k})}{v_{\max}}\right|^2$$

$$= \frac{m_\parallel W}{2\hbar^2 a \pi^2}\left[k_F a - \frac{\sin 2k_F a}{2}\right] , \tag{18}$$

$$k_F = \begin{cases} 0, & \mu - \Delta(\mu) < 0 \\ \dfrac{1}{a}\cos^{-1}\left[\dfrac{-\mu + \Delta(\mu) + W}{W}\right], & 0 < \mu - \Delta(\mu) < 2W \\ \dfrac{\pi}{a}, & \mu - \Delta(\mu) > 2W . \end{cases} \tag{19}$$

Note that $\Delta(\mu) = 0$ for $0 < \mu < 2W$. We find numerically that, as long as $\Gamma(u) < \mu$, this approximation is excellent.

When the chemical potential exceeds the miniband width, although unoccupied (k_x, k_y) states get filled, $\mathbf{v}_z(\mathbf{k})$ of these new states on the Fermi surface does not change (see Fig. 1). Thus the effective carrier density n^* along the superlattice axis remains the same. Furthermore, $\Gamma(\mu)$ remains unchanged when $\mu > 2W$, reflecting the constant density of states. These two effects lead to a conductivity which is independent of μ when $\mu > 2W$.

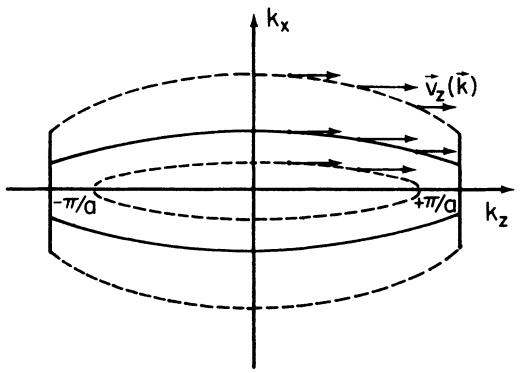

FIG. 1. A schematic drawing of a cross section of the Fermi surface when $\mu > 2W$ or $\mu < 2W$. Many particles on the Fermi surface have finite velocities along the superlattice axis. The sum of the absolute values of these velocities is independent of μ when $\mu > 2W$.

We now present our results. We fix the typical value of the free parameter of our model $\lambda_0 = n_i \mid c \mid^2$ by fitting to Deveaud *et al.*'s experimental value for the hole mobility, 900 $\text{cm}^2/\text{V s}$ at $T = 15$ K, $a = 40$ Å, and $n_0 = 10^{17}$ cm^{-3}.

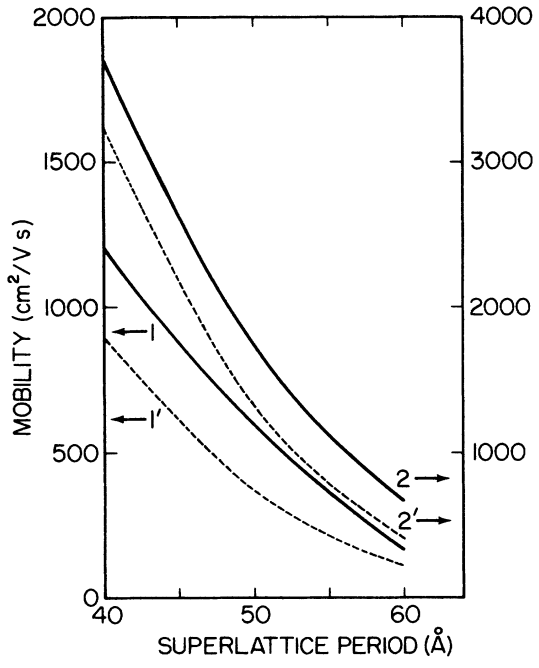

FIG. 2. Dependence of the hole mobility on the superlattice period a. The solid and dashed lines are, respectively, numerical and analytical (Eq. 16) results. The lines 1 and 1' are for $(\lambda, n) = (2.3\lambda_0, 0.3n_0)$ and the lines 2 and 2' are for $(\lambda, n) = (\lambda_0, 0.1n_0)$. The results for $a > 50$ Å are unreliable since $v_F(\mu)\tau(\mu) < a$. The difference between solid and dashed lines shows the failure of the quasiparticle approximation.

These two values of λ_0 and n_0 will be our reference values for impurity and carrier densities. We study superlattices whose widths of GaAs and AlGaAs layers are the same. Since the heavy- and light-hole subband coupling leads to a larger in-plane effective mass, the in-plane mass $m_{\parallel}$ is taken to be the average of GaAs heavy-hole masses normal and parallel to the superlattice axis. The electron (as against the holes) minibands in Ref. 2 have widths of the order of 100 meV and, as such, obey the standard transport theory.

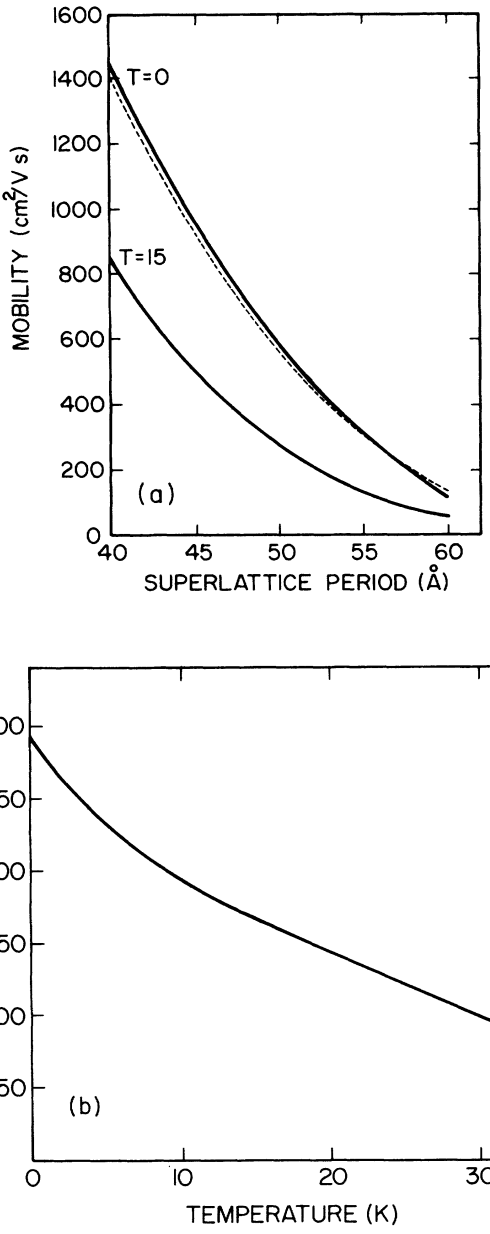

FIG. 3. (a) Dependence of the hole mobility on the superlattice period a for $(\lambda, n)=(\lambda_0, n_0)$. The solid lines are numerical results for $T=0$, 15 K. The dashed line is the analytical result obtained from Eq. (16) at $T=0$. For $a>50$ Å results are unreliable since $v_F(\mu)\tau(\mu)<a$. (b) Temperature dependence of the hole mobility at $a=40$ Å.

In Fig. 2 we show the dependence of the hole mobility on the superlattice period a for $(\lambda, n)=(2.3\lambda_0, 0.3n_0)$ and $(\lambda_0, 0.1n_0)$. The value λ can be increased from λ_0 by introducing more disorder. We see that the mobility obtained using the quasiparticle approximation deviates significantly from the exact numerical result. Thus we conclude that the quasiparticle approximation is unreliable when λ is increased and/or n is decreased. At these densities the mean free paths are still larger than the superlattice periods. We find that at $a=40$ Å, $W[v_z(\mu)/v_{\max}]=5.4$ meV and $\Gamma(\mu)=2.9$ meV for curves 1 and 1′. For curves 2 and 2′ these values are $W[v_z(\mu)/v_{\max}]=3.9$ meV and $\Gamma(\mu)=0.9$ meV. Above $a\sim 50$ Å the Bloch picture breaks down, so the results shown are not reliable. We believe that localization controls transport in these systems for $a>50$ Å, which is consistent with the findings of Ref. 2.

Figure 3(a) displays dependence of the hole mobility on the superlattice period a for $\lambda=\lambda_0$ and $n=n_0$. We find the condition $\Gamma(\mu)<\mu$ to be satisfied for all the results shown in Fig. 3(a). Thus our calculation shows an excellent agreement between the numerical and analytical results. As the superlattice period a increases, the mobility becomes smaller because both m_z and $\Gamma(\mu)/\mu$ increase. At $a=50$ Å the reduction due to the increase of $\Gamma(\mu)/\mu$ is about 30% of the value at $a=40$ Å. Thus a simple formula for mobility $\mu=e\tau/m_z$, where τ is a constant, would be wrong by a factor of 2 due to the quasiparticle corrections discussed in this paper. Figure 3(b) shows the temperature dependence of the hole mobility. We observe that the value at $T=15$ K is different from the $T=0$ value by as much as 40%. This is because the magnitude of the chemical potential is comparable to k_BT.

Figure 4 displays how the conductivity depends on the carrier density. As we have already anticipated from Eq. (16), the conductivity shows a flat dependence on μ for $\mu>2W$. The reason that the conductivity drops for $\mu>2W$ is because $\Delta(\mu)>0$ above the bandwidth.

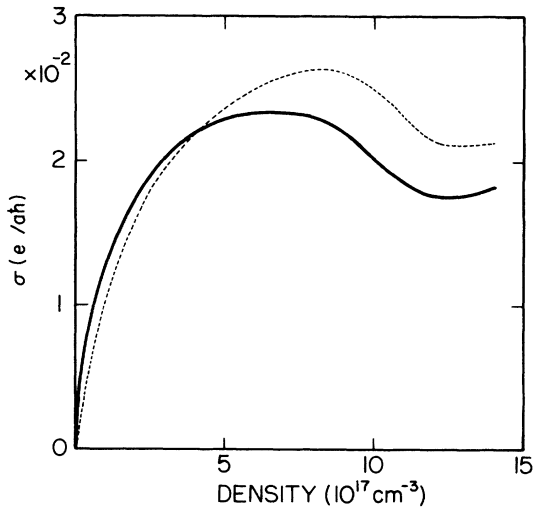

FIG. 4. Dependence of the hole conductivity on the carrier density, at $T=0$ and $\lambda=2.6\lambda_0$. The dashed and solid lines are analytical and numerical results. At $n\sim 8\times 10^{17}$ cm^3 the miniband becomes filled. The period is $a=45$ Å.

Before concluding, we want to emphasize the many approximations made in our theory which should be taken as the zeroth-order transport theory for diffusive miniband transport. In the next order, localization effects will be important even for $l > a$ (i.e., before the Ioffe-Reggel criterion is satisfied) due to the maximally crossed Langer-Neal diagrams left out of our calculations. Thus the actual experimental mobilities can be lower than our calculated theoretical results due to these weak localization corrections. We have also neglected phonon scattering effects which are important in GaAs at higher temperatures (> 100 K) where the polar optical-phonon scattering dominates. The impurity-renormalization effects included in this paper are much less important for electronic miniband transport in superlattices due to the lighter mass of electrons. We find that localization effects dominate electronic transport by the time the quasiparticle corrections treated in this paper are significant (around $a \approx 100-120$ Å).

In conclusion, our study shows that for transport in superlattice minibands the quasiparticle approximation can be unreliable because $\Gamma(\mu) > \mu$. In addition, we find that as the period of the superlattice increases the ratio $\Gamma(\mu)/\mu$ grows substantially, resulting in a reduction of the mobility. Also, since the Fermi energy is small the carriers become nondegenerate already at low temperatures, leading to a significant temperature dependence of the mobility. Another interesting feature is that the conductivity shows very little dependence on the carrier density when the chemical potential exceeds the miniband width.

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