Bloch oscillations and dynamic conductivity of a superlattice

Yu. V. Kopaev

P. N. Lebedev Physics Institute, Russian Academy of Sciences, 117924 Moscow, Russia

S. N. Molotkov

Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russia

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There is an interrelation among the Bloch frequency, the negative differential conductivity, and the generation of oscillations in a superlattice in an electric field. The dynamic conductivity of the superlattice remains negative even at frequencies near the Bloch frequency.

When an ideal crystal is placed in a constant and uniform electric field, an electron at the bottom of the band begins to accelerate. It reaches the boundary of the Brillouin zone and then is reflected by Bragg diffraction to the opposite face of the Brillouin zone. Because of the negative effective mass, the energy of the electron begins to decrease, the electron reaches the bottom of the band, and the process repeats itself. Such oscillations occur at a characteristic Bloch frequency $\Omega_B = eEd/\hbar$, where d is the lattice constant.[1] The finite motion of the electron in **k** space leads to a bounded motion in coordinate space and thus to a quantization of the electron spectrum, with a level separation $\hbar\Omega_B = eEd$ (a so-called Stark ladder).[2,3]

It follows that, if there is no scattering, the system will not conduct a constant electric current, because of the finite nature of the motion. A scattering will lead to a disruption of the Bloch oscillations (the system will become current-conducting), and it will be essentially impossible to observe such oscillations (and the quantization of the spectrum) in 3D crystals.

The idea of superlattices was first proposed by Keldysh,[4] who in the same paper reached the conclusion that these superlattices would have a descending current–voltage characteristic. Esaki and Tsu[5] later proposed a more practical method for implementing this idea, through a variation of the composition or doping. In superlattices, because of the narrow allowed band (a miniband), an electron can traverse an energy interval spanning the entire band without undergoing collisions. In such systems, Bloch oscillations (and a Stark quantization) may be realized. It has also been suggested[5] that Bloch oscillations in superlattices be used to generate microwaves.

However, as was subsequently demonstrated experimentally,[6] Bloch oscillations are not responsible for the generation of oscillations and the descending region of the current–voltage characteristic. Several questions accordingly arise:

1. How is the generation frequency related to the frequency of the Bloch oscillations (the Stark ladder)?

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2. Is the negative differential conductivity associated with "latent" Bloch oscillations in the system?

3. Up to what frequencies is a generation of oscillations possible (i.e., up to what frequencies does the negative differential conductivity persist)?

Attempts have been made[7,8] to clarify these questions through the use of semiclassical description of the dynamics of electrons. Along that approach, however, it is not possible to completely establish the relationship among the negative differential conductivity, the Bloch frequency, and the band properties of the superlattice. The quantum description in terms of the nonequilibrium Keldysh technique[9] makes it possible, in our view, to take a deeper look at the relationship among the quantization of the spectrum, the negative differential conductivity, and the dynamic response of the system. The analysis below reveals the following:

1. In the steady state, the generation frequency is not directly related to the frequency of Bloch oscillations.

2. The successive "shutting" of conducting channels through the superlattice with increasing voltage due to the finite widths of the miniband and of the band in the electrodes is responsible for the negative differential conductivity.

3. The real part of the differential conductivity exhibits a dispersion at frequencies which are multiples of the Bloch frequency, $\Omega_{Bn}=n\cdot\Omega_B$ ($n=1,2,\ldots,N$, where $N\gg 1$ is the number of Stark levels in the superlattice), and remains negative up to frequencies $N\cdot\Omega_B$ which are well above the Bloch frequency Ω_B.

We consider a 1D superlattice of identical tunneling-coupled quantum wells. This assumption is not of fundamental importance for our approach, since the general scheme makes it possible to incorporate a longitudinal motion of the electron and to deal with superlattices with a complex unit cell. These simplifications are necessary only for finding a result in analytic form. We will assume below that the superlattice is connected to metal bands (electrodes).

The spectrum of an isolated superlattice (one not connected to banks) can be found by solving the eigenvalue problem for the Hamiltonian

$$H_{sl}=\sum_{k=1}^{N} c_k^+ c_k \varepsilon_0+\sum_{|i-j|=1} T_{ij} c_i^+ c_j . \qquad (1)$$

Here ε_0 is a level in an isolated well, N is the number of wells in the superlattice, T_{ij} is the matrix element for a jump between neighboring wells, and c_i^+ is a creation operator in the ith quantum well. We assume for simplicity that there is only a single level in an isolated well. In a constant and uniform electric field, Hamiltonian (1) should be supplemented with a term

$$\sum_{k=1}^{N} \frac{ek}{N} V c_k^+ c_k ,$$

where V is the constant voltage across the superlattice, and e is the charge of an electron. Incorporating this term leads to a shift of the bottom of the kth well and level into an isolated well, in such a way that the energy of the level takes the form $\varepsilon_k = \varepsilon_0 + ekV/N$ (in the case of a single level in a well, this is an exact representation, as follows from the properties of the translation operator in an electric field[10]). When there are several levels, there is also a shift of the level with respect to the bottom of the well, due to a change in the shape of the well in the field. This effect arises only in the second order of a perturbation theory in the field. In the case of equal quantum wells, the spectrum of the superlattice should be found from the self-consistent solution of the Schrödinger and Poisson equations.

In our simplified case, a systematic account of the jump leads to the solution of a linear system of $N \times N$ equations. From the solution we find the spectrum and wave function of an isolated superlattice. We find it more convenient to work in terms of a Green's function. For Hamiltonian (1), the Green's function is

$$g_{ij}^R = \sum_{\lambda=1}^{N} \frac{a_{i\lambda} \cdot a_{j\lambda}^*}{\omega - \varepsilon_\lambda + i0}, \tag{2}$$

$$i,j = 1, \ldots, N,$$

where ε_λ is the spectrum of the superlattice with allowance for the tunneling coupling between wells and the electric field, λ is the index of the eigenvalue, and $a_{i\lambda}$ is the amplitude of the wave function in well i corresponding to the λth eigenvalue.

We describe the tunneling coupling between the banks and the superlattice by means of the Hamiltonian

$$H_T = \sum_p [T_{Lp} c_1^+ c_{Lp} + T_{Lp}^* c_{Lp}^+ c_1 + T_{Rp} c_N^+ c_{Rp} + T_{Rp}^* c_{Rp}^+ c_N], \tag{3}$$

where $c_{L,Rp}^+$ are operators in the left and right banks, p is a continuous parameter which describes the spectrum in the banks (e.g., a quasimomentum), and $T_{L,Rp}$ are tunneling matrix elements between the banks and the superlattice. The current operator can be written in the symmetric form[11]

$$\hat{I}(t) = -\frac{ie}{2\hbar} \sum_p \{[T_{Lp} c_1^+ c_{Lp} - T_{Lp}^* c_{L_p}^+ c_1] + [T_{Rp} c_{Rp}^+ c_N - T_{Rp}^* c_N^+ c_{Rp}]\}. \tag{4}$$

To answer the questions raised above, we need to calculate the static current–voltage characteristic and the small-signal response to a small alternating voltage at a constant voltage V [the dynamic conductivity $\sigma(V,\Omega)$]. The static current–voltage characteristic can be found by averaging current operator (4) (see, for example, Refs. 12 and 13):

$$I = \frac{2\pi e}{\hbar} \int d\omega \Gamma_L(\omega) \Gamma_R(\omega) |G_{1N}^R(\omega)|^2 [f_L(\omega) - f_R(\omega)]. \tag{5}$$

Here $f_{L,R}$ are distribution functions in the left and right banks, with chemical potentials μ_L and μ_R; $\mu_L - \mu_R = eV$; and $G_{1N}^R(\omega)$ is the exact Green's function of the superlattice incorporating the tunneling coupling with the banks which describes the propagation of an electron from well 1 to well N:

$$G^R_{1N}(\omega)=\frac{g^R_{1N}(\omega)}{\mathrm{Det}^R}, \tag{6}$$

$$\mathrm{Det}^R=(1-|T_L|^2 g^R_L g^R_{11})(1-|T_R|^2 g^R_R g^R_{NN})-|T_L|^2|T_R|^2 g^R_{1N} g^R_{N1} g^R_L g^R_R,$$

where $g^R_{11,NN}$ are the retarded Green's functions in wells 1 and N in an isolated superlattice, $g^R_{L,R}$ is the Green's function in the banks,

$$g^R_{L,R}(\omega)=\frac{1}{\omega-\varepsilon_{L,Rp}+i0}, \tag{7}$$

$\varepsilon_{L,Rp}$ is the spectrum in the banks, and, finally,

$$\Gamma_{L,R}(\omega)=\pi\sum_p |T_{L,Rp}|^2\delta(\omega-\varepsilon_{L,Rp}) \tag{8}$$

describes the rates of escape into the banks. Equation (6) incorporates multiple scattering in the superlattice. In addition, because of the tunneling coupling with the banks, states in the superlattice become quasisteady. It is for this reason that a current can flow through the lattice.

The interaction with the banks has two effects: a shift of the levels in the minibands and the onset of damping. If the tunneling coupling with the banks is weak, it follows from (6) that pole singularities in $G^R_{1N}(\omega)$ arise at energies $\omega\simeq\varepsilon_\lambda+i\gamma_\lambda$, where ε_λ are the levels in the minibands in an isolated superlattice, and γ_λ is the damping due to escape into the banks (the level width is $\gamma_\lambda\approx\Gamma_L+\Gamma_R$; for a single quantum well this is an exact equality[12]). Consequently, the Green's function in (6) can be written

$$G^R_{1N}\simeq\sum_{\lambda=1}^{N}\frac{a_{1\lambda}\cdot a^*_{N\lambda}}{\omega-\varepsilon_\lambda+i\gamma_\lambda}, \tag{9}$$

where $a_{1,N\lambda}$ is the amplitude in wells 1 and N for level ε_λ in the superlattice. If the wells are weakly coupled with each other, the spectrum in the minibands is almost identical to the levels in the individual wells. In other words, with the levels numbered appropriately we have $\varepsilon_\lambda\simeq\varepsilon_i$ $(\varepsilon_k=\varepsilon_0+keV/N, k=1,2,\ldots N)$.

We finally find [we are assuming a zero temperature; in this case we have $f_{L,R}(\omega)=\theta(\mu_{L,R}-\omega)$]

$$I\simeq 2\pi e\hbar\sum_\lambda\int_{\mu_R}^{\mu_L}\Gamma_L(\omega)\Gamma_R(\omega)\frac{|a_{1\lambda}|^2|a_{N\lambda}|^2}{(\omega-\varepsilon_\lambda)^2+\gamma_\lambda^2}\,d\omega. \tag{10}$$

At low voltages, expression (10) can be put in the form

$$I\simeq\frac{2\pi e^2}{\hbar}V\sum_\lambda |T_\lambda(\mu)|^2, \tag{11}$$

where the transmission coefficient for energy level λ in the miniband is

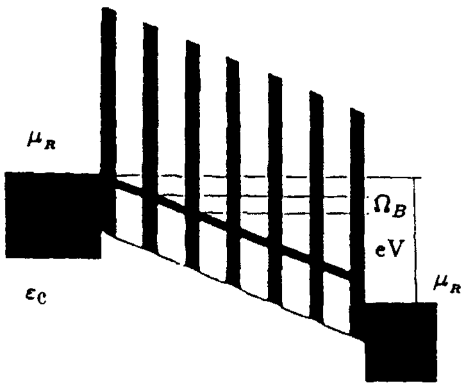

FIG. 1.

$$|T_\lambda(\mu)|^2\Gamma_L\Gamma_R\frac{|a_{1\lambda}|^2|a_{N\lambda}|^2}{(\mu-\varepsilon_\lambda)^2+\gamma_\lambda^2}.$$

We have also noted that in the limit $V=0$ the chemical potentials satisfy $\mu_L=\mu_R=\mu$. It is simple to verify that the descending region of the current–voltage characteristic begins at voltages $V\simeq(\mu_L-\varepsilon_c)/e$ (Fig. 1). Beginning at these voltages, the only contribution to the current comes from those levels in the superlattice which lie below μ_L but above the bottom of the conduction band of the bank, ε_c (Fig. 1). As the voltage V increases, the next energy level in the superlattice finds itself below the bottom of the conduction band, ε_c. The current channel associated with this level stops working, since we have $\Gamma_L(\omega)\equiv 0$ at $\omega<\varepsilon_c$ [see Eq. (8)]. On the descending region of the current–voltage characteristic we have

$$I\simeq\frac{2\pi e^2}{\hbar}\sum_\lambda |T_\lambda(\varepsilon_\lambda)|^2\frac{\mu_L-\varepsilon_c}{(eV/N)}. \tag{12}$$

The last factor here is essentially the number of levels in the interval $\varepsilon_c<\varepsilon_\lambda<\mu_L$.

The finite width of the band in the banks and the miniband is thus responsible for the negative differential conductivity. The negativity of the conductivity stems from the Stark ladder.

We now wish to find the dynamic conductivity, i.e., the response to a weak alternating signal $u(t)$ against the background of a constant voltage V. The perturbation Hamiltonian is

$$\delta H=\sum_{k=1}^{N} e\,\frac{k}{N}\,u(t)c_k^+c_k+\sum_p eu(t)c_{Rp}^+c_{Rp}. \tag{13}$$

For definiteness, we assume that the potential is zero at the left bank. In this case the alternating component of the current can be written as follows, by analogy with Ref. 12:

$$i(t)=\int \sigma(t-t')u(t'), \tag{14}$$

$$\sigma(t-t')=\frac{e^2}{2\hbar}\left\langle \hat{I}(t)\left[\sum_k \frac{k}{N} c_k^+(t')c_k(t')+\sum_p c_{Rp}^+(t')c_{Rp}(t')\right]\right\rangle .$$

In taking an average over the Keldysh contour we should single out the retarded component of the polarization operator. Going through calculations like those of Ref. 12, we find the expression

$$\sigma(\Omega)=\frac{e2}{2\hbar}\int d\omega 2i\sum_{k=1}^{N}\frac{k}{N}\{[\Gamma L(\Omega+\omega)f_L(\Omega+\omega)G_{1k}^A(\Omega+\omega)G_{1k}^A(\omega)$$

$$-\Gamma_L(\omega)f_L(\omega)G_{1k}^R(\Omega+\omega)G_{1k}^R(\omega)]$$

$$-[\Gamma_R(\Omega+\omega)f_R(\Omega+\omega)G_{1k}^A(\Omega+\omega)G_{1k}^A(\omega)$$

$$-\Gamma_R(\omega)f_R(\omega)G_{1k}^R(\Omega+\omega)G_{1k}^R(\omega)]\}$$

$$-i\,[\Gamma_L(\Omega+\omega)+\Gamma_L(\omega)]\sum_{k=1}^{N}\frac{k}{N}[G_{1k}^<(\Omega+\omega)G_{k1}^A(\omega)+G_{1k}^R(\Omega+\omega)G_{k1}^<(\omega)]$$

$$+i\,[\Gamma_R(\Omega+\omega)+\Gamma_R(\omega)]\sum_{k=1}^{N}\frac{k}{N}[G_{Nk}^<(\Omega+\omega)G_{kN}^A(\omega)+G_{Nk}^R(\Omega+\omega)G_{kN}^<(\omega)]$$

$$-2i\,[\Gamma_R(\Omega+\omega)f_L(\Omega+\omega)-\Gamma_R(\omega)f_L(\omega)]\,\frac{1}{\Omega}\,[G_{NN}^R(\Omega+\omega)-G_{NN}^A(\omega)]$$

$$-2[\Gamma_R(\Omega+\omega)f_L(\Omega+\omega)-\Gamma_R(\omega)f_L(\omega)]\,\frac{1}{\Omega}\,-\,[G_{1N}^R(\Omega+\omega)G_{N1}^A(\omega)]$$

$$\times[\Gamma_L(\Omega+\omega)+\Gamma_L(\omega)-\Gamma_R(\Omega+\omega)+\Gamma_R(\omega)]. \quad (15)$$

Terms of the type

$$\sum_p g_{Rp}^R(\Omega+\omega)|T_{Rp}|^2 g_{Rp}^R(\omega)$$

have been omitted from (15). Such terms vanish if we ignore the energy dependence of the density of states in the banks. Here $G_{1k}^<$ is the Keldysh Green's function, for which the following expression can be derived:

$$G_{1k}^<=\frac{1}{|\mathrm{Det}|^2}\{[g_{11}^R|T_L|^2 g_L^< g_{1k}^A+g_{1N}^R|T_R|^2 g_R^< g_{Nk}^A]\,[1-g_R^R|T_R|^2 g_{NN}^R]$$

$$+g_{1N}^R|T_R|^2 g_R^R\,[g_{NN}^R|T_R|^2 g_R^< g_{Nk}^A+g_{1N}^R|T_R|^2 g_R^< g_{Nk}^A]\}. \quad (16)$$

We now consider the response in the voltage region corresponding to the descending part of the current–voltage current characteristic. To simplify the analysis we assume that the voltage V is so high that there are no levels at energies below μ_R (Fig. 1). In this case we

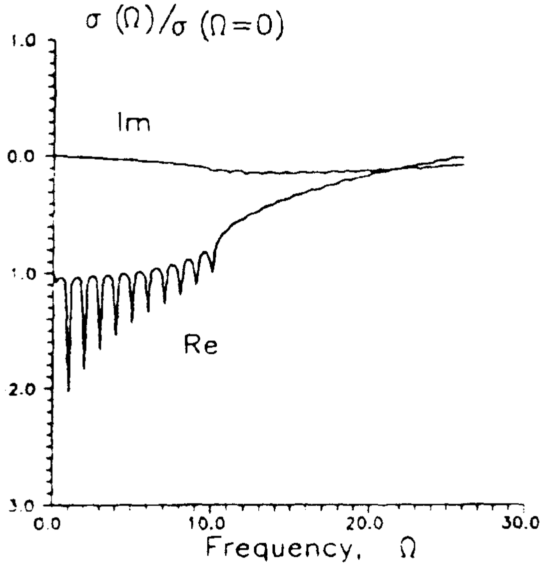

FIG. 2. Dynamic conductivity of the superlattice as a function of the frequency. The calculations used the parameter values $(\mu_L-\varepsilon_c)/\Omega_B=20$, and $\gamma_\lambda/\Omega_B=\text{const}=0.01$.

have $f_R(\varepsilon_\lambda)\equiv 0$, and all terms other than the first two in (14) are irrelevant. In addition, we have $\Gamma_L(\omega)=\Gamma_L=\text{const}$ at $\omega>\varepsilon_c$ and $\Gamma_L(\omega)\equiv 0$ at $\omega<\varepsilon_c$. We can thus write the differential conductivity in the form

$$\sigma(V,\Omega)=2i\,\frac{e^2}{\hbar}\sum_{\lambda,\lambda'}\frac{|a_{1\lambda}|^2|a_{N\lambda'}|^2}{[\Omega-(\varepsilon_{\lambda'}-\varepsilon_\lambda)-i(\gamma_{\lambda'}-\gamma_\lambda)]}$$

$$\times\int d\omega\left\{\Gamma_L(\omega+\Omega)f_L(\omega+\Omega)\left[\frac{1}{\omega-\varepsilon_\lambda-i\gamma_\lambda}-\frac{1}{\omega+\Omega-\varepsilon_{\lambda'}-i\gamma_{\lambda'}}\right]\right.$$

$$\left.-\Gamma_L(\omega)f_L(\omega)\left[\frac{1}{\omega-\varepsilon_\lambda+i\gamma_\lambda}-\frac{1}{\omega+\Omega-\varepsilon_{\lambda'}+i\gamma_{\lambda'}}\right]\right\}. \qquad (17)$$

The summation in (17) is over only those levels which lie in the energy interval $\varepsilon_c<\varepsilon_{\lambda,\lambda'}<\mu_L$. Analysis shows that at large bias voltages (Fig. 1) the real part of the conductivity at zero frequency is negative (the imaginary part is correspondingly zero), and it approaches zero, remaining negative, as

$$\mathrm{Re}\,\sigma(V,\Omega\to\infty)\simeq-\frac{e^2}{2}\frac{\Gamma_L}{\Omega}\sum_{\lambda,\lambda'}|a_{1,\lambda}|^2|a_{N,\lambda'}|^2. \qquad (18)$$

Figure 2 shows the frequency dependence of the conductivity in the case in which γ_λ is a constant (Γ_L) and is independent of the level index, and in which we also have $\varepsilon_\lambda\simeq\hbar\Omega_B\lambda$. This corresponds to a very narrow miniband (weakly coupled quantum wells). For simplicity, we have assumed that $|a_{1,\lambda}|^2|a_{N,\lambda'}|^2$ is a constant (independent of λ). This simplification is sufficient for a qualitative analysis; in general, it would be necessary to solve the problem of finding the spectrum and damping through a solution of a system of linear equations.

The real part of the differential conductivity thus remains negative even at frequencies above the Bloch frequency $\Omega_B = eEd/\hbar$ and at multiples of it, $\Omega = k\Omega_B$. The negativity of this conductivity is in no way related to the Bloch frequency. The negative conductivity of this frequency implies that a generation of radiation is possible (if there is a corresponding resonator). The frequency of the radiation will be determined by the parameters of the external circuit.

There is an analogy with generation in a laser and in a superlattice with a negative differential conductivity at a large bias voltage. For generation to become possible in a laser, a population inversion must be set up. This means that the states in the conduction band (for definiteness, we are considering a semiconductor laser), with a relatively high energy, must have a higher population than states in the valence band, with a relative low energy. In this case the absorption coefficient (the conductivity at the corresponding frequency) becomes negative. In a superlattice with a large bias voltage (Fig. 1), the population of the levels in the interval $[\mu_L, \varepsilon_c]$ is higher than for levels with energies below ε_c. This point can be understood at a qualitative level. A quantitative analysis of the population, on the other hand, will require determining the Keldysh Green's function $G^<_{kk}$ in an arbitrary well. For this problem it is a straightforward matter to find an expression analogous to (16) (where necessary, the contribution of inelastic processes to the damping γ_λ should be added). In this sense, the physical reason for the generation is totally unrelated to the Bloch frequency (Stark quantization). For example, placing a superlattice in a charged plane capacitor, but without electrical connection between the superlattice and the plates, results in a Stark quantization of levels. Obviously, however, no radiation will occur, since states in the superlattice are stationary states. The negative differential conductivity is directly responsible for the generation of oscillations. The physical reason for the generation is essentially the same as in laser systems. Generation can occur if a population inversion is set up. This can be done either by connecting to electrodes (as discussed above; in this case there is steady-state generation because of the constant replenishment of the population) or through a temporary scattering of carriers into upper levels (by means of laser light, for example) into a superlattice which is isolated (but naturally in an electric field). In this case generation occurs in a transient regime, until the populations become equal (through relaxation or recombination). In a sufficiently strong field, in which the degree of localization of the electrons in an individual well is high, the most intense radiation will obviously occur at the frequency corresponding to the energy difference in neighboring wells. This radiation is frequently called "Bloch oscillations."[14]

We note that, as was shown in Ref. 10 on the basis of simple qualitative considerations, the radiation intensity in an infinite superlattice of identical wells is zero. In a finite superlattice, the intensity is determined by the distribution functions in the outermost wells. Steady-state generation is thus possible only in a finite superlattice, and it is essentially an edge effect.

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