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Theory of electron transport in a superlattice miniband

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Abstract. Electron transport in a superlattice miniband with dissipative and random environments is considered on the basis of a general theory of open quantum systems. We obtain the analytical dependence of the electron drift velocity on applied electric field, which contains a region with negative differential conductivity. The results are compared with experimental data and the predictions of other theories.

1. Introduction

Electron transport in semiconductor superlattices has attracted considerable attention over many years because these structures are rich in interesting effects [1–12]. The main ones are the many types of electron localization in one-dimensional models [11–13] and the possibility of negative differential conductivity (NDC) in strong electric fields [1, 2]. The existence of NDC was confirmed both by numerical calculations by means of Monte Carlo techniques [3–5] and by experiments [6]. But there is no universally accepted theoretical explanation for this phenomenon. According to Esaki and Tsu [1], NDC is caused by the electron motion within the miniband including a region of momentum where the electron effective mass is negative. The measurements of the peak of the drift velocity and the critical electric field carried out in [6] are in partial agreement with the work described in [1] as well as with the more sophisticated theory proposed in reference [8] and based on the balance equations. However, both theories predict the unlimited increasing of the drift velocity peak with increasing of the superlattice miniband width, whereas the experiment [6] indicates a saturation of this dependence when the miniband width is more than 100 meV.

Another mechanism producing NDC is connected with transfers between Wannier–Stark levels in the inclined miniband [2]. This theory predicts a linear dependence of the critical electric field and a superlinear dependence of the drift velocity peak on the miniband width. At large miniband width these predictions fail to agree with the experimental data [6].

The aim of present paper is the construction of a microscopical theory of electron transport in superlattices in the presence of a constant electric field, taking into consideration optical phonon scattering and impurity scattering. Usually, theoretical investigations have been carried out either in the framework of the semiclassical Boltzmann equations in the τ -approximation [7] or by means of the numerical solution of the balance equations [8–10]. In these investigations it was supposed that the electron distribution function is Maxwellian or Fermi with the electron temperature T_e . Thereby, the electron temperature was considered as a parameter which did not correlate with the level of electron velocity fluctuations. However, the variances of the electron velocity fluctuations along the field direction and

transversely can be totally different [14, 15]. This is of particular importance for the study of superlattices which are strongly anisotropic structures.

In the present work we try to circumvent the necessity for making any assumptions about the electron distribution function along the field direction (and along the superlattice axis), and derive the equations for generating functions of momentum fluctuations. In reference [12] this approach made it possible to consider the electron transport in purely one-dimensional superlattices and to find a new type of dynamical localization in such structures. In the present work we take into account the transverse degrees of freedom as well. On the basis of the theory of open quantum systems proposed in references [15–17], we obtain an analytical expression for the dependence of the drift velocity on the applied electric field. In addition, we analyse the dependences of the drift velocity peak and the critical electric field on the miniband width, and compare our results with experimental data and the predictions of other theories.

2. Theory

The Hamiltonian of the system under study in the tight-binding approximation is

$$H = \frac{\Delta}{2} \left[1 - \cos\left(\frac{p_z(t)d}{\hbar}\right) \right] + \frac{p_{\perp}^2}{2m} - eEz(t) + H_{ep} + H_{ei} + H_p \quad (1)$$

where $\mathbf{r}(t)$ and $\mathbf{p}(t)$ are the electron position and momentum operators, respectively, $\mathbf{p}_{\perp} = (p_x, p_y)$, d is the period of the superlattice, Δ is the miniband width, and E is the electric field strength. Also

$$H_{ei} = L^{-3/2} \sum_k U_k e^{i\mathbf{k}\cdot\mathbf{r}(t)}$$

and

$$H_{ep} = L^{-3/2} \sum_k Q_k(t) e^{i\mathbf{k}\cdot\mathbf{r}(t)}$$

describe the electron–impurity interaction and the electron–phonon interaction, respectively. Here L is the linear spatial size of the system, U_k is the Fourier transform of the impurity potential, and $Q_k(t)$ is a variable relating to the phonon heat bath with the unperturbed Hamiltonian H_p .

For the case of polar optical phonons, which provide the main mechanism of scattering in polar semiconductors at sufficiently high temperature, the Hamiltonian of the electron–phonon interaction has the form

$$H_{ep} = e \left(\frac{2\pi\hbar\Omega_0}{L^3\kappa^*} \right)^{1/2} \sum_k \frac{i}{k} (b_k(t) e^{i\mathbf{k}\cdot\mathbf{r}(t)} - b_{-k}^+ e^{-i\mathbf{k}\cdot\mathbf{r}(t)}). \quad (2)$$

Here $1/\kappa^* = 1/\kappa_{\infty} - 1/\kappa_0$, where κ_{∞} and κ_0 are the hf and static permittivities of the crystal, respectively, Ω_0 is the optical phonon frequency, and $b_k^+(t)$ and $b_k(t)$ are the phonon creation and annihilation operators, respectively.

It should be noticed that, in view of the relation $|eEd| \ll \Delta_g$, where Δ_g is a forbidden miniband width, we do not take into account the transfers between minibands. Also, we consider the non-degenerate limit in which the Pauli principle can be ignored.

To describe the electron motion along the superlattice axis direction (the z -axis) without making any assumptions about the electron distribution function, we consider the generating function of the momentum's z -projection fluctuations:

$$F_n(t) = \langle \exp\{in p_z(t)/\hbar\} \rangle$$

where $n = 1, 2, \dots$. A steady value of $(F_1)_0$ will define the electron drift velocity along the z -axis:

$$V_d = \langle \dot{z}(t) \rangle = \frac{\Delta d}{2\hbar} \left(\left\langle \sin \left(\frac{p_z(t)d}{\hbar} \right) \right\rangle \right)_0 = \frac{\Delta d}{2\hbar} \text{Im}(F_1)_0. \quad (3)$$

Angle brackets mean simultaneously thermally averaging and quantum mechanically averaging, as well as averaging over impurity configurations.

We can write Heisenberg's equation for the generating function $F_n(t)$ as follows:

$$\dot{F}_n(t) + L^{-3/2} \sum_k \frac{2}{\hbar} \sin \left(\frac{k_z d}{2} n \right) \left(Q_k(t) + U_k \exp \left\{ i\mathbf{k} \cdot \mathbf{r}(t) + i \frac{nd}{\hbar} p_z(t) \right\} \right) = in\Omega_B F_n(t) \quad (4)$$

where $\Omega_B = eEd/\hbar$ is the frequency of the Bloch oscillations.

According to the general theory of open quantum systems [15–17], this equation can be rewritten as

$$\begin{aligned} \dot{F}_n(t) + \int \frac{d^3k}{(2\pi)^3} \sin \left(\frac{k_z d}{2} n \right) \int_{-\infty}^t dt_1 \left((M_k(t, t_1) + \Phi_k) \right. \\ \left. \times \left\langle \frac{i}{\hbar} [\exp\{i\mathbf{k} \cdot \mathbf{r}(t) + indp_z(t)/\hbar\}, \exp\{-i\mathbf{k} \cdot \mathbf{r}(t_1)\}]_- \right\rangle \right. \\ \left. + \varphi_k(t, t_1) \left\langle \frac{1}{2} [\exp\{i\mathbf{k} \cdot \mathbf{r}(t) + indp_z(t)/\hbar\}, \exp\{-i\mathbf{k} \cdot \mathbf{r}(t_1)\}]_+ \right\rangle \right) \\ = in\Omega_B F_n(t) \end{aligned} \quad (5)$$

where $\varphi_k(\tau)$ and $M_k(\tau)$ are the linear response function and the correlation function of the unperturbed phonon variables, respectively, and Φ_k is the correlation function of the impurity potentials. For the case of scattering on polar optical phonons and on charged impurities, these functions have the forms [15, 18]

$$\begin{aligned} \varphi_k(\tau) &= \frac{4\pi\Omega_0 e^2}{k^2 \kappa^*} \sin(\Omega_0 \tau) \theta(\tau) \\ M_k(\tau) &= \frac{2\pi\hbar\Omega_0 e^2}{k^2 \kappa^*} \cos(\Omega_0 \tau) \coth \left(\frac{\hbar\Omega_0}{2T} \right) \\ \Phi_k &= \frac{2e^4 n_i^*}{\pi \kappa_0^2 (k^2 + r_0^{-2})^2} \end{aligned} \quad (6)$$

where $\theta(\tau)$ is the Heaviside step function, r_0 is the screening radius, $n_i^* = \sum_\alpha n_\alpha Z_\alpha^2$, n_α is the concentration of impurities of branch α , and Z_α is its charge.

In the case of weak electron–phonon coupling and weak electron–impurity scattering we can neglect the interaction effects on the period of the memory time of equation (5). This is a good approximation for polar semiconductors [15]. Then, to calculate the commutators, we will consider the time evolution of the position operators to be the following:

$$\mathbf{r}_\perp(t) = \mathbf{r}_\perp(t_1) + \tilde{\mathbf{V}}_\perp(t_1)(t - t_1) \quad (7)$$

$$z(t) = z(t_1) + \frac{\Delta d}{\hbar\Omega_B} \sin \left(\frac{\Omega_B(t - t_1)}{2} \right) \sin \left(\frac{p_z(t_1)d}{\hbar} - \frac{\Omega_B(t - t_1)}{2} \right) \quad (8)$$

where $\tilde{\mathbf{V}}_\perp$ is a random velocity in the transverse degrees of freedom. Using the operator expression

$$e^{\hat{A}} e^{\hat{B}} = \exp \left\{ \hat{A} + \int_0^1 d\xi e^{\xi\hat{A}} \hat{B} e^{-\xi\hat{A}} \right\}$$

and equations (7), (8), we obtain

$$\begin{aligned}
& \left\langle \frac{i}{\hbar} [\exp\{i\mathbf{k} \cdot \mathbf{r}(t) + indp_z(t)/\hbar\}, \exp\{-i\mathbf{k} \cdot \mathbf{r}(t_1)\}]_- \right\rangle \\
&= \frac{2}{\hbar} \sum_{m=-\infty}^{m=\infty} \exp\left\{-i\frac{m\Omega_B}{2}\tau\right\} \left\langle \exp\left\{i\frac{(m+n)d}{\hbar}p_z(t)\right\} \right\rangle \\
&\quad \times J_m \left\{ \frac{2\Delta}{\hbar\Omega_B} \sin\left(\frac{\Omega_B\tau}{2}\right) \sin\left(\frac{k_z d}{2}\right) \right\} \langle \exp\{i\mathbf{k}_\perp \cdot \tilde{\mathbf{V}}_\perp \tau\} \rangle \\
&\quad \times \left[\sin\left(\frac{k_z d}{2}(m+n)\right) \cos\left(\frac{\hbar k_\perp^2}{2m}\tau\right) + \cos\left(\frac{k_z d}{2}(m+n)\right) \sin\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right]
\end{aligned} \tag{9}$$

$$\begin{aligned}
& \left\langle \frac{1}{2} [\exp\{i\mathbf{k} \cdot \mathbf{r}(t) + indp_z(t)/\hbar\}, \exp\{-i\mathbf{k} \cdot \mathbf{r}(t_1)\}]_+ \right\rangle \\
&= \sum_{m=-\infty}^{m=\infty} \exp\left\{-i\frac{m\Omega_B}{2}\tau\right\} \left\langle \exp\left\{i\frac{(m+n)d}{\hbar}p_z(t)\right\} \right\rangle \\
&\quad \times J_m \left\{ \frac{2\Delta}{\hbar\Omega_B} \sin\left(\frac{\Omega_B\tau}{2}\right) \sin\left(\frac{k_z d}{2}\right) \right\} \langle \exp\{i\mathbf{k}_\perp \cdot \tilde{\mathbf{V}}_\perp \tau\} \rangle \\
&\quad \times \left[\cos\left(\frac{k_z d}{2}(m+n)\right) \cos\left(\frac{\hbar k_\perp^2}{2m}\tau\right) - \sin\left(\frac{k_z d}{2}(m+n)\right) \sin\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right].
\end{aligned} \tag{10}$$

Here $\tau = t - t_1$ and $J_m(x)$ are Bessel functions.

Substituting these relations into equation (5), we are led to a system of equations for the generating functions $F_n(t)$ ($n = 1, 2, \dots$):

$$\dot{F}_n(t) + \sum_{m=-\infty}^{m=\infty} G(n, m) F_{m+n}(t) = in\Omega_B F_n(t) \tag{11}$$

where the ‘collision term’ $G(n, m)$ is defined by the expression

$$\begin{aligned}
G(n, m) = & \int \frac{d^3k}{(2\pi)^3} \frac{2}{\hbar} \sin\left(\frac{k_z d}{2}n\right) \int_0^\infty d\tau \left\{ \frac{2}{\hbar} (M_k(\tau) + \Phi_k) \right. \\
& \times \left[\sin\left(\frac{k_z d}{2}(m+n)\right) \cos\left(\frac{\hbar k_\perp^2}{2m}\tau\right) + \cos\left(\frac{k_z d}{2}(m+n)\right) \sin\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right] \\
& + \varphi_k(t, t_1) \left[\cos\left(\frac{k_z d}{2}(m+n)\right) \cos\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right. \\
& \left. \left. - \sin\left(\frac{k_z d}{2}(m+n)\right) \sin\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right] \right\} \\
& \times J_m \left[\frac{2\Delta}{\hbar\Omega_B} \sin\left(\frac{k_z d}{2}\right) \sin\left(\frac{\Omega_B\tau}{2}\right) \right] \exp\left(-i\frac{m\Omega_B}{2}\tau\right) \langle \exp\{i\mathbf{k}_\perp \cdot \tilde{\mathbf{V}}_\perp \tau\} \rangle. \tag{12}
\end{aligned}$$

The generating function of the velocity fluctuations in the transverse degrees of freedom $\langle \exp\{i\mathbf{k}_\perp \cdot \tilde{\mathbf{V}}_\perp \tau\} \rangle$ requires detailed analysis. In the present work we first assume these fluctuations to be Gaussian, so

$$\langle \exp\{i\mathbf{k}_\perp \cdot \tilde{\mathbf{V}}_\perp \tau\} \rangle = \exp\left\{-\frac{k_\perp^2}{2} \langle \tilde{\mathbf{V}}_\perp^2 \rangle \tau^2\right\} \tag{13}$$

where $\langle \tilde{V}_\perp^2 \rangle = \langle \tilde{V}_x^2 \rangle = \langle \tilde{V}_y^2 \rangle$, and, second, we neglect the transverse heating, i.e. assume that $\langle \tilde{V}_\perp^2 \rangle = T/m$. These assumptions simplify the calculations significantly, but give qualitatively correct results.

For the case of weak electron–phonon and electron–impurity interactions, for which the condition $|G(n, m)/\Omega_B| \ll 1$ is fulfilled, we obtain

$$\dot{F}_n(t) + \gamma_n F_n(t) + G(n, -n) = i n \Omega_B F_n(t) \quad (14)$$

where $\gamma_n = G(n, 0)$ plays the role of a damping rate, while $G(n, -n)$ defines the steady state of the generating function $F_n(t)$:

$$(F_n)_0 = \frac{G(n, -n)}{i n \Omega_B}. \quad (15)$$

The electron drift velocity (3) is proportional to the imaginary part of the function $(F_1)_0$:

$$V_d = \frac{\Delta d}{2\hbar} \left\langle \sin\left(\frac{p_z d}{\hbar}\right) \right\rangle_0 = \frac{\Delta d}{2\hbar} \text{Im}(F_1)_0 = -\frac{\Delta d}{2\hbar \Omega_B} \text{Re} G(1, -1). \quad (16)$$

The ‘collision term’ $G(1, -1)$ can be found after substitution of $n = 1$ and $m = -1$, the expressions for the correlation functions and the response function (6), and the generating function of transverse velocity fluctuations (13) into equation (12), and integrating with respect to τ .

As a result, we obtain the expression for the dependence of the electron drift velocity on the applied electric field:

$$\begin{aligned} V_d = V_0 \frac{1}{\sqrt{\Theta}} \sum_l l \int_0^{k_D} dk_z \int_0^{k_D} dk_\perp \frac{1}{k^2} J_l^2 \left\{ \frac{\Delta}{\hbar \Omega_B} \sin\left(\frac{k_z d}{2}\right) \right\} \\ \times \left((N_0 + 1) \left(\exp\left\{ -\frac{1}{2} \frac{m(\omega_k + \Omega_0 - l\Omega_B)^2}{k_\perp^2 T} \right\} \right. \right. \\ \left. \left. - \exp\left\{ -\frac{1}{2} \frac{m(\omega_k + \Omega_0 + l\Omega_B)^2}{k_\perp^2 T} \right\} \right) \right. \\ \left. + N_0 \left(\exp\left\{ -\frac{1}{2} \frac{m(\omega_k - \Omega_0 - l\Omega_B)^2}{k_\perp^2 T} \right\} - \exp\left\{ -\frac{1}{2} \frac{m(\omega_k - \Omega_0 + l\Omega_B)^2}{k_\perp^2 T} \right\} \right) \right. \\ \left. + \frac{\alpha k^2 r_0^2}{(k^2 r_0^2 + 1)^2} \left(\exp\left\{ -\frac{1}{2} \frac{m(\omega_k - l\Omega_B)^2}{k_\perp^2 T} \right\} - \exp\left\{ -\frac{1}{2} \frac{m(\omega_k + l\Omega_B)^2}{k_\perp^2 T} \right\} \right) \right). \end{aligned} \quad (17)$$

Here $k^2 = k_z^2 + k_\perp^2$, $N_0 = [\exp(\hbar\Omega_0) - 1]^{-1}$, and

$$V_0 = \frac{m e^2 \Omega_0 d^2}{2\sqrt{\pi} \hbar^2 \kappa^*}.$$

Also, $\Theta = 2md^2T/\hbar^2$ is the normalized temperature, $\omega_k = \hbar k_\perp^2/2m$, and

$$\alpha = \frac{e^2 n_i^* \kappa^* r_0^2}{\pi^2 \kappa_0^2 \hbar \Omega_0}$$

is a parameter describing the relationship between the constants of the electron–phonon and electron–impurity interactions.

3. Discussion

The formula obtained, equation (17), admits a clear interpretation. In the limit of low temperature (or if we neglect velocity fluctuations in the transverse degrees of freedom), the factor

$$\frac{\sqrt{m}}{\hbar\sqrt{2\pi T}} \exp\left\{-\frac{1}{2} \frac{m(\omega_k \pm \Omega_0 \pm l\Omega_B)^2}{k_{\perp}^2 T}\right\} \rightarrow k_{\perp} \delta(\hbar\omega_k \pm \hbar\Omega_0 \pm \hbar l\Omega_B)$$

represents the energy conservation law for the scattering.

Thus, we can interpret the electron transport as the transition of an electron from one level of a Wannier–Stark ladder to another. The electron absorbs (emits) a phonon or scatters on an impurity and goes to another energy level. The difference between the phonon energy and the distance between the levels (or the complete energy distance in the case of impurity scattering) transfers to transverse degrees of freedom (or is covered by transverse degrees of freedom). The drift motion is determined as the difference between electron motions downwards (along the electric field) and upwards (against the field). Therewith, the Bessel functions modify the matrix elements of the electron–phonon and electron–impurity interactions in the presence of a superlattice potential. Thermal fluctuations in the transverse degrees of freedom transform the δ -functions to exponents.

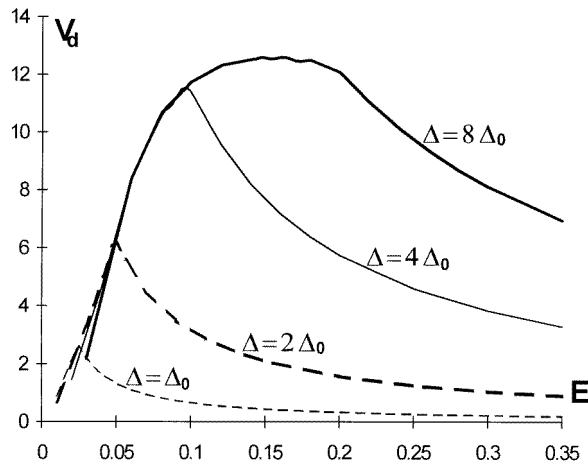


Figure 1. The dependence of the drift velocity on the applied constant electric field for different miniband widths at the temperature $T = 300$ K.

In figure 1 the dependences of the electron drift velocity on the applied electric field for different miniband widths Δ at the lattice temperature $T = 300$ K are presented. As may be seen, at weak field this dependence is similar for different miniband widths. This is because in this case the electron scatters on a phonon and goes to another Wannier–Stark level well before the Bragg reflection occurs. This leads to ohmic current–voltage characteristics at weak field as well. At stronger fields Bragg reflections take place, and this gives rise to a region with negative differential conductivity. It is clear that the critical field increases with increase of the miniband width. At the significant miniband width Δ , the curves of the fall region became smoother. This is explained by the modification of the matrix elements of the electron–phonon and electron–impurity interactions in the presence of the superlattice potential. One can even see weak oscillations due to the Bessel functions in the modified

matrix elements.

The drift velocity is normalized to V_0 , which is equal to $8 \times 10^5 \text{ cm s}^{-1}$ for a superlattice produced from GaAs/AlAs with the period $d = 5.7 \times 10^{-7} \text{ cm}$. The electric field is normalized to $E_0 = \hbar^2/2emd^3$, which is equal to 30 kV cm^{-1} under the same conditions. The values of the miniband width are expressed in units of $\Delta_0 = \hbar^2/2md^2 = 1.76 \times 10^{-2} \text{ eV}$.

For these samples, the constant α determining the relationship between the constants of the electron–impurity interaction and the electron–phonon one is equal to $6 \times 10^{-24} n_i^*$, where n_i^* is measured in cm^{-3} , i.e. is very small at usual concentrations of impurities. Therefore, impurity scattering contributes to electron transport at extremely low temperature and for weak fields only.

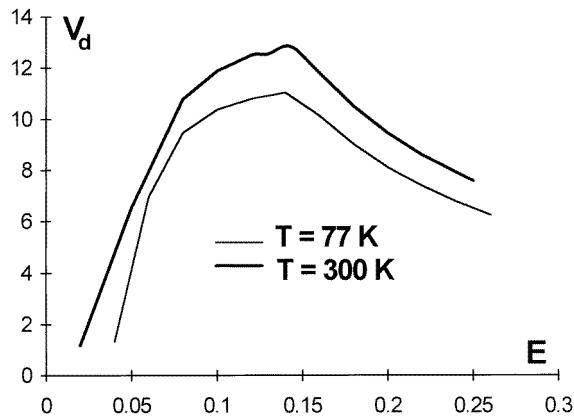


Figure 2. The dependence of the drift velocity on the applied constant electric field for different temperatures at the miniband width $\Delta = 6\Delta_0$.

In figure 2, the dependence of the drift velocity on the applied field is shown for different temperatures at the miniband width $\Delta = 6\Delta_0$. As one can see, the curves for different temperatures are similar, which is in agreement with experimental data [6].

To compare the results of the present work with experimental data as well as with the predictions of other theories, we demonstrate the dependences of the values V_p/d and $E_c d$ on the miniband width in figure 3 and figure 4, respectively. Here E_c is the field at which the region with negative differential conductivity has its onset and V_p is the drift velocity at this field.

One can see from figure 3 that our results are qualitatively in agreement with experimental data. All other theories predicted unlimited increasing of the ratio V_p/d as the miniband width increases. The deviation from this behaviour was explained by the possibility of electron transfer to another miniband. However, we have shown that this phenomenon can be explained by significant modification of matrix elements of the electron–environment interaction at large Δ in the framework of a single-miniband model. The quantitative agreement can be improved by taking into account carrier heating in the transverse degrees of freedom by means of a procedure proposed in [15].

The dependence of the critical field on the miniband width is presented in figure 4. The experimental data for the large miniband width provided a reason for not accepting the model proposed in reference [2], wherein the negative differential conductivity was caused by transfers between Wannier–Stark levels in the inclined miniband. Our model is

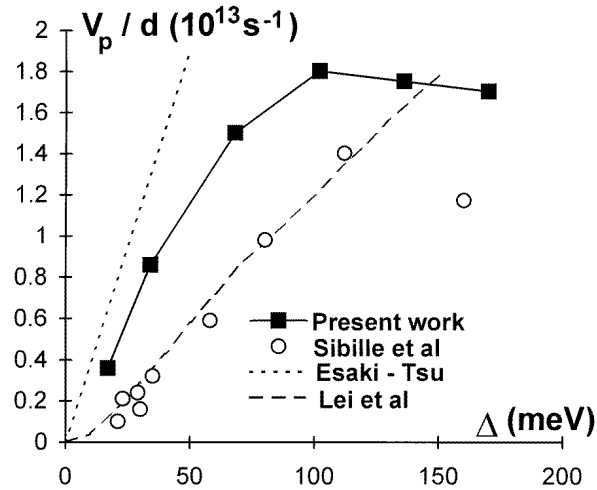


Figure 3. The dependence of the ratio of the velocity drift peak to the superlattice period on the miniband width at the temperature $T = 300$ K.

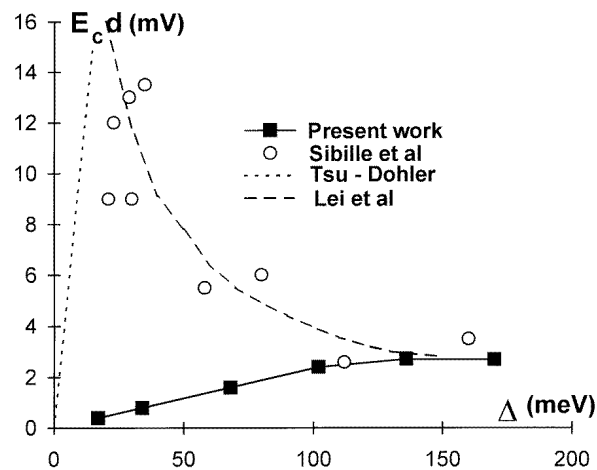


Figure 4. The dependence of the product of the critical electric field and superlattice period on the miniband width at the temperature $T = 300$ K.

analogous to that of Tsu and Dohler, but our points at large Δ are in excellent agreement with experiments. The deviation at small Δ is significant, but, as is evident from the foregoing, increasing of the critical field with increasing of the miniband width would appear reasonable. Moreover, it should be mentioned that the experimental measurement of the field value presents considerable difficulties, due to the lead effects. It cannot be too highly stressed that for the experimental points at small Δ there is a wide scatter of data. In addition, the larger value of the critical field obtained from the experiment could be associated with insufficient interface quality of the experimental samples. Anyway, the measurements of the current value are more plausible, but in this case (figure 3) our data are near to the experimental ones.

4. Conclusions

We now give a brief summary of the main results of this work.

We have considered quantum transport in the semiconductor superlattice in the framework of the single-miniband model. On the basis of the general theory of open quantum systems, the non-Markovian equations for the generating function of momentum fluctuations are derived for the case of the presence of a constant electric field as well as dissipative and random environments. This has made it possible to obtain the analytical dependence of the electron drift velocity on the applied electric field. This dependence demonstrates the most significant feature of the electron transport in superlattices, namely, the region with negative differential conductivity. Our results have been compared with the predictions of other theories and the experimental data. The values of the drift velocity at the point of transition to the regime of negative differential conductivity show qualitative agreement with well-known experimental results [6] and, moreover, explain the experimental data at large miniband widths. The critical electric field increases linearly with the miniband width because the negative differential conductivity is caused by the Bragg reflection in the inclined miniband. At the large width Δ , our results are in good agreement with experimental data.

It should be noticed that the quantitative agreement can be improved by means of a self-consistent treatment of kinetic and fluctuation processes in superlattices on the basis of the approach proposed in reference [15]. In addition, the equations obtained in the present paper can be generalized to include the presence of magnetic or time-dependent electric fields.

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