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Phonon-limited near equilibrium transport in a semiconductor superlattice

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Abstract. — This paper deals with transport properties at low applied electric field in a one-dimensional semiconductor superlattice. Two scattering processes are considered: deformation potential and polar optical modes. Umklapp corrections are made using a plane-wave method giving envelope wavefunctions. The collision time approximation is discussed in the present context. The method is applied to GaAs/GaAlAs superlattice systems and the mobility tensor is computed as a function of the superlattice period.

Introduction. — Molecular beam epitaxy and, to some extent, other epitaxial techniques have enabled new artificial materials such as one-dimensional superlattices to be built. These have been realized for example in lattice matched semiconductor systems such as Ga_{1-x}Al_{x}/GaAs [1] or InGaAs/GaAsSb [2]. Esaki [3] originally proposed the following mechanism: if a regular superlattice of period $d$ in the $z$ direction is built, it follows a subsystem of path $2 \pi /d$ in reciprocal space; during transport mechanisms, electrons may be subjected to « Bloch oscillations » if the mean free path is such that the Brillouin zone edge can be reached without collision for an electron starting from $k_z = 0$. A large number of papers have been devoted to this subject [4], but fundamental aspects remain a matter of controversy [5]. However, it is not necessary to introduce Bloch oscillations into the non-linear analysis of the transport problem; the special features of the band along $k_z$ may be at the origin of the instability. Transport along $k_z$ is only possible in true superlattices and not in M.Q.W. (Multiple Quantum Wells) structures in which transport has essentially a bidimensional character.

Growth of superlattices leads to novelties in the derivation of transport coefficients. The first novelty is the high anisotropy of the band structure which increases the difficulty in summing over $k$ wavevectors. A second novelty lies in the selection rules. In [6], we gave rough estimates of such effects with the deformation-potential scattering. In the present paper, a general derivation of the mobility tensor will be given. This method has some advantages over the classical Kronig-Penney ordinary derivation. A direct use of it is the knowledge of the envelope wavefunction Fourier coefficients. Once we have the matrix elements of the electron-phonon interactions, we can derive a general collision time $\tau(k)$:

$$\tau(k) = \left( \sum_k W(k \rightarrow k') \right)^{-1} \quad (1)$$

in which $W(k \rightarrow k)$ is the scattering-out probability per unit time. For elastic scattering processes a relaxation time $\tau_R(k)$ can be defined:

$$\tau_R(k) = \left( \sum_k W(k \rightarrow k') (1 - \cos(k, k')) \right)^{-1} \quad (2)$$

The cosine terms are the scattering-in terms. For inelastic processes, (1) is the basis of a general derivation of some transport equation, but (2) cannot be used in the mobility derivation. However, we shall see that a simple use of $\tau$ gives essential behaviour of the mobility tensor.

In the first part, we describe a simplified method to obtain both band structure and envelope wavefunction coefficients. In the second part, we discuss the solution of Boltzmann equation and the method based upon (1). In part 3, we apply the solutions given in
parts 1 and 2 to a simple case (deformation potential scattering). In the fourth part, the central problem of polar optical phonon scattering is dealt with in two steps: first the derivation of \( \tau(\mathbf{k}) \), then an Umklapp correction factor. All the practical applications of the theory are made with the popular GaAs/GaAlAs system which seems, up to now, the best suited to the present set of hypotheses.

1. Band structure and envelope wavefunctions. — Pseudo-potential methods have proved to be very useful in the calculation of III-V band structures [7]. They have been applied to one special superlattice with a rather simple primitive cell, the GaAs/AlAs monolayer and a few layer superlattices [8, 9]. Tight binding [10] methods have also been used, but they cannot give useful parameters for transport problems. If electrons (or holes) are not too far from band extrema, Kronig-Penney (K.P.) models give a reasonable solution [11] provided that the primitive cell contains a sufficient number of atoms of each species. The K.P. model has been improved to take into account \((\Gamma)-(X)\) or \((\Gamma)-(L)\) mixing according to the nature of the respective band extrema in each material [12].

The Kronig-Penney model (K.P.), however, does not lead to tractable envelope wavefunctions. We propose an alternative model based on the same set of hypotheses as K.P., but which gives the envelope wavefunctions in a directly available expansion. A first approximation we must make is to assume a mean effective mass for the whole material. Effective mass jumps lead to theoretical complexities, not within the scope of the present paper [13]. Electrons are then supposed to belong to \((\Gamma)\) valleys of both materials and are only subjected to a crenel potential as described in figure 1. Thus the one-electron Hamiltonian is:

\[
H = H_0 + V_{\text{SL}}(z)
\]

in which \( V_{\text{SL}}(z) \) has the period of the superlattice and can be expanded as a Fourier series:

\[
V_{\text{SL}}(z) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{iGz}.
\]

For a crenel potential having the parameters shown in figure 1:

\[
V_{\text{SL}} = \frac{b}{d} W \sin \left( \frac{Gb/2}{Gb/2} \right).
\]

Now, the wavefunction solution of (3) can be written in the form:

\[
\Psi(k) = \varphi_0(k) \sum_{\mathbf{G}} C_{\mathbf{G}} e^{i\mathbf{Gz}}
\]

in which \( \varphi_0(k) \) is the effective-mass solution of \( H_0 \).

As in the K.P. model, only the plane wave part of \( \varphi_0(k) \) is considered. We therefore have the following relations,

\[
\frac{1}{L} \int_0^L \varphi_0^* \varphi_0 e^{-iGz+ig\mathbf{z}} dz = \delta_{G0}.
\]

in which \( L \) is the sample width in the \( z \) direction and \( \delta \) the Kronecker symbol. Analysis of (7) with a general form of \( \varphi_0(k) \) reveals that its structure on an atomic scale only influence high-order \( C_{\mathbf{G}} \) coefficients. Combining (6) and (3) with the orthogonality relations (7), we obtain the secular system of equations

\[
C_{\mathbf{G}} \varepsilon_0(k_z + G) + \sum_{\mathbf{G'}} V_{\mathbf{G'}-\mathbf{G}} = \varepsilon(k) C_{\mathbf{G}}
\]

in which \( \varepsilon_0(k) \) is given by the effective mass approximation. Then the total energy \textit{versus} wavevector relation is given by:

\[
\varepsilon(k) = \frac{h^2 k_\perp^2}{2m^*} + \varepsilon_{\|}(k_\perp)
\]

in which \( k_\perp = \sqrt{k_x^2 + k_y^2} \) is the projection of \( k \) in the layer plane and \( k_\| = k_z \). The system (8), truncated to a given order can deliver \( \varepsilon_{\|}(k_\perp) \) (eigenstates of the system) and a set of \( C_{\mathbf{G}} \) coefficients (eigenvectors of the system), e.g. minibands and envelopes. A problem may arise with respect to which order we can truncate to obtain a reasonable accuracy. We have made a test to compare the above model, which we shall call the plane-wave model (P.W.), with K.P. Note that both models have exactly the same set of physical hypotheses, but have different mathematical methods.

To give an example of some results obtained by the P.W. method and to compare these with K.P., we have taken the GaAs/Ga\(_{1-x}\)Al\(_x\)As system. The crenel amplitude \( W \) is a function of the aluminium percentage \( x \):

\[
W = 1.06 x.
\]

The mean effective mass is also a function of \( x \):

\[
m^* = (am^*_1 + bm^*_2)/d
\]

in which \( m_1 = 0.067 \) (GaAs) and \( m^* = m^*_1 + 0.083 m^*_2 \) (ternary compound). There is no evident physical
basis for such an arithmetic average (11), but it seems to be the best way to avoid the difficulties introduced by effective mass jumps in (3).

This approximation is quite reasonable when the effective masses are not too different, which is the case here. However, when electrons are confined in the wells the approximation (11) leads to a somewhat too large effective mass, the most probable value being close to $m^*_1$. Some results are shown in figures 2 and 3. Miniband structures have been derived as a function of $x$ for different crenel configurations, as a function of $d$ (Fig. 2) and with $a = b$ and $a = 3 b$ ($x = 0.3$) in figure 3. We shall see that the width of the lowest lying miniband is an important parameter in transport properties of such superlattices (miniband widths are given in meV in figure 2). Neither K.P. nor P.W. give tractable analytical expressions of $\varepsilon_{ij}(k)$ and so, some authors have thus proposed a phenomenological form of the band [4]:

$$\varepsilon_{ij}(k) = \Delta (1 - \cos (k \parallel d)). \quad (12)$$

Even if this expression does not fit well the results of P.W., the important features of the analytical derivation arise through the bandwidth $2 \Delta$.

In the following text, $2 \Delta$ will designate the bandwidth along $k \parallel$ even as a result of computer P.W. solutions.

We now compare the results of P.W. and K.P. for the chosen GaAs/AlAs system. Figure 4 shows the maximum difference in the miniband energies of the K.P. and P.W. derivations as a function of the number of $C_G$ coefficients (P.W.). We also find that the convergence is faster for a smaller lattice period $d$ as a result of the wavefunction smearing out the wells. Further analysis also shows that $C_G$ values converge to stable values at any $k_r$. Thus an interesting form of the envelope is obtained by (6), which is very useful both for transport studies, and other physical quantities.

2. Solution of transport equation near equilibrium. — The Boltzmann transport equation (B.T.E.) is the basic equation for most transport studies in semiconductors. To derive the mobility tensor, a weak

![Figure 2](image_url)
electric field $E$ is applied to the system. The electron distribution function $f(k)$ is a solution of:

$$\frac{eE}{\hbar} \cdot \nabla f(k) =$$

$$= \sum_{k',\alpha} (W_s(k' \rightarrow k) f(k') - W_o(k \rightarrow k') f(k)). \quad (13)$$

We note that $\alpha$ is an interaction index, many collision processes being involved, but a single band approach is taken in the present context. A solution of (13) is not evident in the superlattice case, mainly because of inelastic processes. A general discussion of a solution of (13) is out of the scope of the present paper, but appendix A to which the reader is referred, discusses the drastic approximations we have made to go sufficiently far in the mobility derivation. The simplified expression of the distribution function near equilibrium is:

$$f(k) = \bar{f}(\epsilon) - \frac{eE}{\hbar} \cdot \nabla \bar{f}(\epsilon) \tau(k) \quad (14)$$

in which $\tau(k)$ is just the expression given by (1), $\bar{f}(\epsilon)$ the equilibrium distribution function.

In (A), the expression (14) is shown to be correct for deformation potential scattering at high temperatures and not too inexact for polar optical scattering in typical cases. However, note that (14) is not the direct solution of (13) since of neglects the first terms in the sum of the second part of (13), i.e. scattering-in. This has been discussed extensively in the case of polar optical scattering in III-V compounds by Rode [14].

Two main collision processes will be studied in the present paper: acoustic phonons (deformation potential), and polar optical phonons. The associated $W$ are given by:

**acoustic**:

$$W_s = \frac{2\pi}{\hbar V} \left( N_\sigma + \frac{1}{2} \pm \frac{1}{2} \right) \frac{E_s^2 \hbar \omega_\sigma}{2 \rho_\sigma^2} \delta(U^\pm) \delta(k', k, q) \quad (15)$$

**optical**:

$$W_o = \frac{\pi}{\hbar V} \left( N_\sigma + \frac{1}{2} \pm \frac{1}{2} \right) \frac{e^2 \hbar \omega_0}{q^4} \left( \frac{1}{K_\infty} - \frac{1}{K_0} \right) \delta(U^\pm) \delta(k', k, q) \quad (16)$$
in which the following quantities are defined:

\[ N_q = \left( \frac{\exp \frac{\hbar \omega(q)}{k_B T} - 1}{\exp \frac{\hbar \omega(q)}{k_B T}} \right)^{-1} = \text{equilibrium phonon statistics}, \]

\[ E_1 = \text{deformation potential}, \]

\[ \delta(U^\pm) = \delta(e(k') - e(k) \pm \hbar \omega(q)) = \text{energy conservation quantity}, \]

\[ K_{\alpha}, K_{\nu} = \text{static and optical dielectric constants}, \]

\[ \rho, V = \text{material density and volume}, \]

\[ \omega_0 = \text{optical phonon energy} \text{ (long waves)}, \]

\[ I^\pm(k', k, q) = \left| \langle k' | e^\pm iq | k \rangle \right|^2 \]

reducing to \( \delta(k' - k \mp q) \) for N-processes.

To go further in the derivation of any \( f(k) \) (15)-(17), we define a coordinate system and general lines of summation over \( k' \) states:

\[ \sum_{k'} = \frac{V}{(2\pi)^3} \int_0^{2\pi} d\delta' \int_0^\pi \sin\delta' \int_{-\infty}^{\infty} dk' \]

in which \( (k'_\|, \theta') \) are the polar coordinates in the planes normal to \( k'_z \) defined earlier. Each integral in (18) will contain a \( \delta \)-function of the total transfer energy:

\[ U^\pm = \frac{\hbar^2}{2m^*} (k^2_\perp - k^2_z) + e_i(k') - e_i(k) \pm \hbar \omega(q) \]

(19)

in which

\[ q = \pm (k' - k) - G. \]

In Normal-processes \( (G = 0) \) the integration over \( k'_\| \) must be taken as a first step in two simple cases:

(i) \( \hbar \omega(q) \ll \langle \epsilon \rangle \) (almost elastic collisions),

(ii) \( \hbar \omega(q) = \text{constant} \) (optical-phonon scattering)

(20)

in all others cases, the integration processes through the \( \delta \)-function are not clear. The derivation of (18) will imply the following Jacobian:

\[ \frac{\partial U^\pm}{\partial k'_\|} \simeq \frac{\hbar^2}{m^*} k'_\|. \]

(21)

The other novelty of the present problem is the special care devoted to \( I^\pm(k', k, q) \), not reducible to a single Kronecker. A general solution of these integrals can be given as soon as plane wave coefficients are obtained:

\[ I^\pm(k', k, q) = \sum_n A^+_n S(k') C_n(k) \]

(22)

in which

\[ A_n = \sum_p C^+_p S(k') C_n(k). \]

Such solutions are easy to introduce in a computer program and analytical gross features will be made in the very simple case of acoustic phonons in the following section.

3. A simple case : acoustical phonon scattering. — Deformation potential coupling is not very efficient in most III-V compounds compared with polar or piezoelectric couplings [14]. However, as an introductory example, it may be useful to comment on the derivation of \( \tau \) and the related mobility tensor. The order of summation in (18) is chosen as follows: first \( k'_\|, \) then \( \theta' \), then \( k'\perp \). From (21)-(15) and (19)-(20), the following result is straightforward:

\[ \frac{1}{\tau} = \frac{E_i^2 m^*}{2 \pi \rho \omega^2 \hbar^3} T \int \epsilon(k', k'_||) dk'_||. \]

(24)

Note that (24) is more general than equation (8) of [6] since it includes the Umklapp integral. The restriction \( I' \) on the integration domain over \( k'_\| \) is easy to interpret from figure 5 and the comment made in reference [6]. The integral over \( I' \) in (24) can be reduced to 2 \( k_1 \) for normal processes, \( k_1 \) being in general a solution of the following equation:

\[ e_i(k_1) = \epsilon(k) \]

(25)

\( k_1 \) can generally be given as a computer solution in association with P.W. eigenvalues. A simpler solution has been given in [6].

Two interesting limits arise from (24) and phenomenological expressions for \( k_1 \) (see Ref. [6]):

— the bidimensional case in which \( D \) vanishes with \( \Delta \). The surprising result for this case is that \( \tau \) becomes proportional to \( \Delta \). We point out that U-processes \((I_g \neq 1) \) must be introduced in that case;

— the tridimensional case \( (\Delta \) very large, effective mass solution assumed near \( k'_\| = 0 \)). Here, the usual parabolic mean relaxation time is found, for the N-process restriction:

\[ \tau_3D = \frac{\pi \rho \omega^2 \hbar^2}{\sqrt{2} E_i^2 k_B T m^* \sqrt{M}} \epsilon^{-1/2} \]

(26)
Fig. 5. — Representation of constant-energy lines $\varepsilon(k) = \text{const.}$ in the plane $(k_\perp, k_\parallel)$. The domain $D$ is limited by $\varepsilon(k) = 2 \Delta$. Inside $(D)$ there is a limiting zone $(T)$ for $k_\parallel$ component, whereas for $(D')$ all the $k_\parallel$ values in
\[
\left(-\frac{\pi}{d}, +\frac{\pi}{d}\right)
\]
are allowed.

in which $M$ is the effective mass along $k_\parallel$ in the miniband. The usual (3D) relaxation time is found with $m^* M^{1/2}$ instead of $(m^*)^{3/2}$.

Now, the near-equilibrium relaxation-time for N-processes only can be derived from (24), (25) : expressions have already been given in [6].

We define an Umklapp correction factor $\zeta(k)$ which can be deduced from the set of $A_n$ coefficients by (22) (23) :
\[
\zeta(k) = \frac{\tau_a(\text{Umlapp + Normal})}{\tau_a(\text{Normal})}.
\]

Fig. 6. — Representation of the mean Umklapp corrections versus $d$ for acoustic modes. There is a saturation of the effect at large $d$ values.

Fig. 7. — Representation of the near-equilibrium mobility tensor (acoustic modes scattering) versus $d$. Both normal and normal plus Umklapp scattering (dotted line) are seen. Here, we have chosen a symmetric superlattice, and $x = 0.4$ to fix the barrier height.

Fig. 8. — Same representation as figure 5, for optical mode scattering. This case is more complex as inelastic events connect different energies (the difference being constant, $\hbar \omega_0$). Two examples are drawn nearby $2 \Delta + \hbar \omega_0$ and $2 \Delta - \hbar \omega_0$. 
We have performed a numerical computation of \( \zeta(k) \). The main feature is a very weak variation of \( \zeta \) with \( k \). However, the mean value \( \langle \zeta \rangle \) decreases with \( d \) as expected, and may be used as a correcting factor, see figure 6.

Now, we can derive the mobility tensor \( \overline{\mu} \) through (14), (15), (22), (23). Results are shown in figure 7 in which \( \mu_\parallel \) and \( \mu_\perp \) in the acoustic case are represented versus \( d \) for a symmetric superlattice \((a = b)\) made of GaAs and GaAAs as \( T = 300 \) K. The numerical values are normalized to \( \mu_{3D} \) (isotropic material of effective mass \( m^* \)). Two remarks can be made concerning these results:

- \( \mu_\perp \) is lower than \( \mu_{3D} \) (50 %) in the whole range of measurable \( \mu_\parallel \). Then it increases but does not surpass \( \mu_{3D} \) if \( U \)-processes are taken in account.

- \( \mu_\parallel \) exponentially decreases with \( d \). This is clearly seen from equation (12) in [6]; both \( \Delta_1^\parallel \) and \( k_d \) factors contribute to the exponential decrease of \( \mu_\parallel \).

4. Polar optical phonon scattering. — Since in most III-V compounds, the polar-optical phonon scattering is the most important process at room temperature, this section will be the central one. Results are not as simple as for the acoustic case described above since the matrix elements (16) are strongly \( q \)-dependent even at high temperatures. Moreover, the energy conservation requirement connects different energies in \( k \) space (description such as in figure 8). Use of computer techniques cannot be evaded here. The first step of our derivation is to compute \( q_\perp^2 \):

\[
q_\perp^2 = \left| k' - k \mp G \right|^2.
\]

We remark that relevant \( G \) values of the present problem have only \( k_\parallel \) components:

\[
q_\perp^2 = k_\perp^2 + k_d^2 - 2 k_\perp k_d \cos \theta' + (k_\parallel - k_\parallel \mp G)^2.
\]

In (31), \( k_\perp^2 \) and \( k_d^2 \) terms must be computed at \( U^\pm = 0 \). To go further, we make use of the reduced variables:

\[
u = \frac{k_\parallel}{k_\perp}, \quad v = \frac{k_\parallel'}{k_\perp}, \quad g = \frac{G}{k_\perp}, \quad \lambda = k_\perp d, \quad \gamma_1 = \frac{m^* e^2 \omega_0}{h^2 2 \pi K_0} \left( \frac{1}{K_0} - \frac{1}{K_0} \right).
\]

The first step of integration of (16) over \( k' \) is performed through \( \delta(U^\pm) \) (energy relations) so that we have:

\[
\frac{1}{\tau_{po}} = \gamma_1 \int_0^{2\pi} d\theta' \left\{ \int_{-r}^{r} \frac{I^+(k_\parallel, k_\parallel') \left[ N(\omega_0) + 1 \right] dk_\parallel}{q_\perp^2} + \int_{-r}^{r} \frac{I^-(k_\parallel, k_\parallel') N(\omega_0) dk_\parallel}{q_\perp^2} \right\}
\]

in which \( I^\pm \), are given by (22) and depend only on \( \epsilon, k_\parallel', \theta' \) and \( G \).

To go step by step, we shall first derive \( \tau_{po} \) for an \( N \)-process \((I^\pm = 1)\). Thanks to the reduced variables introduced above it follows that:

\[
\frac{1}{\tau_{po}} = \frac{2 \pi \gamma}{k_\perp} \left( N(\omega_0) + 1 \right) \left( 1 + \frac{q_\perp^2}{K_\perp^2} \right)
\]

in which the integrals \( J^\pm \) are given by:

\[
J^\pm = \int_{-r}^{r} \frac{dv}{\sqrt{(1 + K_\perp^2)^2 + 2(1 + K_\parallel^2)(u - v)^2 + (u - v)^4}}
\]

\[
K_\perp = \sqrt{1 + \Omega^* + \epsilon_\parallel(\lambda u) - \epsilon_\parallel(\lambda v)}.
\]

Now, we must determine the limits \( I^\pm \) entering (30)-(32), which are more complex than in part 3. In figure 8, we try to describe what occurs near three critical lines:

(i) \( \epsilon = \Omega = \hbar \omega_0 \) limiting \((D_0)\) and \((D_0')\),

(ii) \( \epsilon = 2 \Delta + \Omega \) limiting \((D_+\) and \((D_+')\),

(iii) \( \epsilon = 2 \Delta - \Omega \) limiting \((D_-\) and \((D_-')\).

In case (i), electrons in \( D_0 \) cannot emit phonons of energy \( \Omega \); this is the classical emission edge. In case (ii), the emission of a phonon will give a new state \( k' \) such that a \( I^+ \) domain in \( k_\parallel \) will be less than \( 2 \pi/d \). In case (iii), the inverse will occur with absorption and a limiting domain \( I^- \) for \( k_\parallel \), but the last case
may or may not exist according to the $2 \Delta$ value with respect to $\Omega$. A summary of all possible cases is given in Table I. Such a table may be used in a general way to find the limits in a computer program, according to $\Delta$, $\Omega$ and $k$ values.

Table I. — Summary of all the possible cases of the electron-optical phonon processes. ($k$) = starting state; ($k'$) = final state. (a) = absorption process, (e) = emission process. $D_0$ and $D_0'$ are separated by $\epsilon = 2 \Delta$ as $D_+ + D_0$ by $\epsilon = 2 \Delta + \Omega$ and $D_-$ and $D_0'$ by $\epsilon = 2 \Delta - \Omega$ (see Fig. 8). $I^0 = (- \pi/d, + \pi/d)$ and $I^\pm$ correspond to the limits of $(D_\pm, D'_\pm)$ on the $k'_\parallel$ axis.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$k'$</th>
<th>Process</th>
<th>Limit</th>
<th>General restrictions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_0$</td>
<td>$D_-$</td>
<td>a</td>
<td>$I^-_\parallel$</td>
<td>$\Omega &lt; 2 \Delta$</td>
</tr>
<tr>
<td>$D_0$</td>
<td>$D'_-$</td>
<td>a</td>
<td>$I^0_\parallel$</td>
<td></td>
</tr>
<tr>
<td>$D_0$</td>
<td>$D_+$</td>
<td>e</td>
<td>$I^+_\parallel$</td>
<td></td>
</tr>
<tr>
<td>$D_0$</td>
<td>$D_-$</td>
<td>a</td>
<td>$I^-_\parallel$</td>
<td>$\Omega &lt; \Delta$</td>
</tr>
<tr>
<td>$D_0$</td>
<td>$D'_+$</td>
<td>e</td>
<td>$I^0_\parallel$</td>
<td>$\Omega &lt; 2 \Delta$</td>
</tr>
</tbody>
</table>

The limiting value $k'_\parallel$ for $k'_\parallel$ is given by $\epsilon_i(k'_\parallel) = \epsilon + \Omega$.

A computer program has been used to derive numerical results from (31)-(32) and table I. In figures 9 and 10, we show two typical examples whose parameters have been deduced from the P.W. results: $a = b = 35 \AA$, $2 \Delta = 38$ meV and 22 meV respectively, with a phonon energy of 27 meV. Three main effects are seen:

— the usual edge at $\epsilon = \Omega$ for any $k$, which is interpreted as the sudden increase of the transition probability as soon as phonons can be emitted ($\epsilon > \Omega$);
— two (or one) adjacent changes of slope at $\epsilon = 2 \Delta + \Omega$ (or $\epsilon = 2 \Delta + \Omega$ only). This has been commented above as the transition between a constant limit in

$$I^\pm(-\frac{\pi}{d} < k'_\parallel < \frac{\pi}{d})$$

and a variable-limit regime ($-k_1 < k'_\parallel < k_1$);
— a neat $k$ dependence when $2 \Delta - \Omega < \epsilon < 2 \Delta + \epsilon$. This is new in comparison with former hypotheses. A model of $\tau_{po}$ can be given in the very flat band to describe the variations of $\tau_{po}$ with $\epsilon$ only.

As made in part 3, the Umklapp correction must be introduced here. The effect is, however, expected to be weaker as the transition probabilities vary as $q^{-2}$. Remarking that:

— the coefficients $A_n$ do not depend on $\theta$;

— the expression of $\epsilon'_i$ can always be replaced by another of $\epsilon_i$, $k'_i$, $k'_\parallel(U^\pm = 0)$, the general result holds:

$$\xi(k) = \frac{\tau_{po}(U + N)}{\tau_p(U)} = \frac{\lambda_0^p(N(\omega_0) + 1) + \lambda_0^e N(\omega_0)}{\sum_0^\infty (\lambda_0^p(N(\omega_0) + 1) + \lambda_0^e N(\omega_0))}$$

(33)
in which:

\[ J_n^\pm = \int_{-1}^{1} \frac{A_n^2 \, dt}{\sqrt{(1 - K^2)^2 + 2(1 + K^2)(u - v + g_1)^2 + (u - v + g_2)^4}} \]  

in which the expressions for \( K^\pm, u, v, \) etc., are the same as (32) and \( A_n \) are given by the plane-wave methods (22).

Numerical results are seen in figure 11. The average value of \( \langle \xi \rangle \) is now closer to 1 than the corresponding value in the acoustic case. This can be interpreted as the integrated value over \( k'_1 \) and \( \theta' \) leads to a term roughly proportional to the inverse of \( |q| \approx G_n \).

Fig. 11. — Umklapp correction \( \langle \xi \rangle \) in optical mode case, versus \( d \).

The final results concern the mobility tensor limited by polar optical phonon scattering at 300 K, which can be related to experimental values of weakly doped materials. A complete computer solution has been obtained from \( a, b, d, x, \) (or \( W \)) to obtain \( \mu_\perp \) and \( \mu_\parallel \).

Normalization to \( \mu_\perp = \mu_\parallel = \mu_{3D} \) at very low \( d \) values is made by the relation \( M = \hbar^2/\Delta d^2 = m^* \) for these values. Agreement is obtained within a few percent. Results are seen in figure 12. The same remarks made about the acoustic phonon scattering are still valid here, namely an exponential variation of \( \mu_\parallel/\mu_{3D} \) becomes larger than 1 even if \( U \)-processes are taken in account. This can be explained by the nature of the average \( m^* \) value used in \( \mu_{3D} \). For \( \mu_\perp \) Umklapp taken apart, the confining effect in the material of lowest effective mass \( (m^*_\perp) \) leads to \( \mu_\perp/\mu_{3D} > 1 \) in the M.Q.W. area \( (m^*_\perp > m^* \) by a factor \( \sim 2 \)). So, for M.Q.W. materials \( (d > 150 \text{ Å}) \), the transverse mobility must become closer to \( m^*_\perp \) than \( m^* \). At the same time, the numerical value of \( \mu_\parallel \) is very low, in the hopping range, and another theory of the mobility is needed (phonon-assisted tunnelling). For example, if \( \mu_{3D} \sim 2000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1} \), we find \( \mu_\parallel \sim 10 \) as soon as \( d = 100 \text{ Å} \).

The validity of the whole procedure cannot be completely asserted in the present case since we made use of equations (14), which are only valid for quasi-elastic collisions. However the procedure seems to be not very far from the exact solution since we considered the exact behaviour of \( \tau_{po} \) with \( k \).

5. Discussion. — We have derived expressions and numerical derivations of the near-equilibrium mobility tensor in a semiconductor superlattice. The present theory is not restricted to the GaAs/GaAlAs system taken here as a commonly used example. However, it is restricted to band structures in which conduction and valence bands do not overlap (as occurs in the InAs/GaSb system). Only two scattering processes have been studied: acoustic modes (deformation potential) and polar optical modes. In both cases, the phonon modes are not perturbed by the
superlattice construction; this is not obvious in the acoustic case, (15), but is easier to infer in the optical case. The present work is a complete calculation taking account of the Umklapp processes. Thus, the shape of the wavefunction is of some importance; a plane wave calculation has been used, (as treated in many textbooks introducing Bloch function properties). We have noted, that an analytical expression of $\tau(k)$ is easy to obtain in the acoustic case but on the contrary, polar optical phonons, being more complex to deal with, do not give simple expressions for $\tau(k)$.

Meanwhile, previous assumptions concerning $\tau(k)$ [4] are not verified in the present context: both the $k_y$ and $\varepsilon$ dependence of $\tau_{\text{opt}}$ are not trivial and can only be determined from a computer solution relative to some integral over $k_y$ (integration over $k_z$ and $\theta'$ being analytically possible). The final results which are averages of the velocity giving the mobility tensor wave not predictable except, perhaps, the exponential dependence of $\mu_{\parallel}$ with $d$. If we try to derive the tunnel current at very low applied voltage in a system of $N$ barriers connected by $N$ resistors, we also find an exponential variation with the barrier width: tunnelling in such a system of barriers is the same as band transport of Bloch waves when the bandwidth tends to zero. However, if too much disorder is added to the system, we expect drastic changes in the results, i.e. a weaker value of the mobility and a critical dependence of the transition between band transport and hopping transport with the amount of disorder. Finally, Umklapp corrections have been made, giving $\sim 100\%$ for acoustic mode, $\sim 30\%$ for optical modes, in agreement with previous rough estimates. The basic explanation of such an effect consists in the zone folding effect applied to the electron system.

The present work can be extended to more complex situations: e.g. multi-band transport (heavily doped materials), hole transport in p-type materials and impurity scattering. However this is out of the scope of the present paper because the description of scattering centres and collision integrals is a separate problem.

Our results can be compared with previous derivations of $\mu_\perp$ for M.Q.W. systems [16]. We find a smaller value of the mobility limited by polar optical modes. Here, even if the transport along $z$ becomes weaker, the electron-phonon system remains classical except that we introduce Umklapp effects. Thus, the reduction of the transverse mobility is not related to the absence of $q_z$ but merely to the somewhat higher collision integrals in quasi-two-dimensional systems as compared with a three-dimensional system. However, such a difference may be counterbalanced by the scattering-in we have neglected above by assuming a simple collision-time expression (scattering-out) of the near-equilibrium distribution function.

Appendix A. General solution of B.T.E. — We look at a general solution of B.T.E. in the superlattice case, near-equilibrium. The best way is to put (13) into the Chambers Budd form [17]:

$$f(k) = \int_{-\infty}^{0} \left( \exp \int_{0}^{k} \frac{d\varepsilon}{\tau(\varepsilon)} \right) \sum_{k'} W(k' - k^*) f(k^*) dt$$

(A.1)

in which:

$$k^* = k - \frac{e}{\hbar} E t.$$  

(A.2)

(A.1) can be solved by successive integration by parts. We do not retain term in each integration which is of a higher-order in $E$.

There remains an expansion of the type:

$$f(k) = \bar{f}(\varepsilon) + \sum_{0}^{\infty} \varphi^{(p)}(k).$$  

(A.3)

Since each term $\varphi^{(p)}$ is linear in $E$; a recurrent relation between $\varphi^{(p)}$ and $\varphi^{(p-1)}$ holds:

$$\varphi^{(p)}(k) = \tau(k) \sum_{k'} W(k' \rightarrow k) \varphi^{(p-1)}(k')$$

(A.4)

$$\varphi^{(0)}(k) = -\frac{eE}{\hbar} \cdot \nabla_k \bar{f}.$$

As pointed out earlier [14], the solution limited to $\varphi^{(0)}$ does not take into account the scattering-in and generally under-estimates the mobility.

We define a first correction tensor $\bar{\tau}_1$ by:

$$\tau E \left( \frac{1}{\tau_1} \right) \nabla_k \bar{f} = \sum_{k'} W(k' \rightarrow k) E. \nabla_k \bar{f} (k') \tau (k').$$  

(A.5)

An approximate distribution function is thus given by:

$$f(k) = \bar{f}(\varepsilon) - \frac{e}{\hbar} E. \nabla_k \bar{f} \bar{\tau}_R.$$  

(A.6)

To go further, it is necessary to suppose some invariance in $(\bar{\tau}_1/\tau_1)$ under a change of axes. This may be assumed for elastic processes, leading to the well known relaxation-time formula:

$$f(k) = \bar{f}(\varepsilon) - \frac{e}{\hbar} E. \nabla_k \bar{f} \tau_R$$  

(A.7)

with $\tau_R$ given by (2).

Thus as a first result we can assert that (14) is strictly valid for deformation potential scattering since $W(k \rightarrow k')$ is independent on $q$ and the cosine term contribution (scattering-in) strictly vanishes when one integrates over $k'$.
For polar optical scattering, we can only estimate the order of magnitude of the correction tensor \( \tau/\tau_1 \) to justify our hypothesis (14). That correction tensor has two components:

\[
\left( \frac{\tau}{\tau_1} \right)_\perp = \sum_{k'} W(k' \to k) \cos \theta \frac{\partial f}{\partial k_\perp} \tau(k') \tag{A.8}
\]

\[
\left( \frac{\tau}{\tau_1} \right)_\parallel = \sum_{k'} W(k' \to k) \frac{\partial f}{\partial k_\parallel} \tau(k') .
\]

The only case in which one of these corrections is important concerns \( \tau/\tau_1 \perp \) when \( \varepsilon_1 > \hbar \omega_0 \), as

\[ W(k' \to k) \sim | k' - k | - 2 . \]

However, the near equilibrium mobility is not affected by such high energies. Further numerical studies of (A.4) in polar optical scattering are in progress, but superlattice mobilities are probably not more enhanced by scattering-in than ordinary polar materials (\( \sim 30 \% \)), and the effect is greater for \( \mu_\perp \) than \( \mu_\parallel \).

References


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