

Formalization for the study of conductivity in multisubband quantum wells

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The linearized Boltzmann equation is established in the case of multisubband quantum wells where elastic and inelastic scattering mechanisms act simultaneously and may induce intersubband transitions. A numerical procedure is proposed to solve this equation even in the case where intersubband transitions are considered. The multisubband screening is also considered, and approximate expressions for the static dielectric functions are given.

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I. INTRODUCTION

The experimental possibilities for obtaining large carrier densities within AlGaIn/GaN quantum wells due to the spontaneous polarization and piezoelectric effects render highly probable that their conductivity results from a multisubband process. In such a case, the theoretical prediction of low-field transport properties becomes difficult since the linearized Boltzmann equation also includes the contribution of interband transitions which drastically complicates its numerical solution. Moreover, the screening effects are determined by all occupied subbands and their description becomes much more elaborate. The first approaches concerning intersubband transitions and screening effects can be found in Refs. 1 and 2 in the case of silicon inversion layers. The role of intersubband coupling and screening on ionized impurity scattering potentials has been developed in Refs. 3 and 4 and was also studied using Monte Carlo simulations as in Ref. 5–7. An analytical approach, using trial wave functions for the determination of the quantum well states, was proposed in the case of AlGaIn/GaN.⁸ However, in this last paper, the first subband only was considered as electronically filled in order to simplify the calculation. The aim of this series of two papers is to determine theoretically the mobility that can be expected in such quantum wells, including therefore extrinsic scattering mechanisms (impurities, lattice defects, interface roughness, etc.) as well as intrinsic mechanisms associated with phonons and carrier-carrier scattering. For doing so, we first establish the linearized Boltzmann equation in the case of a multisubband electronic system submitted to a combination of elastic and inelastic scattering potentials. Then we describe the numerical method we have developed to solve it and give numerical results showing that interband transitions lead to non-negligible effects on the carrier mobility. In the third part, we formally develop the multisubband dielectric response and we show how we have approximately taken into account this formalism for the evaluation of the scattering matrix potentials used in the present mobility calculation.

II. NUMERICAL SOLUTION OF THE LINEARIZED BOLTZMANN EQUATION

A. Linearized Boltzmann equation

We consider a two-dimensional electron gas whose subbands are noted by an index n and whose energy states are given by

$$E_{n,k} = E_n + \frac{\hbar^2 k^2}{2m^*} = E_n + \varepsilon_k. \quad (2.1)$$

In Eq. (2.1) we implicitly make the assumption that each subband is characterized by the same effective mass. The kinetic Boltzmann equation is obtained by considering that in the presence of applied fields the electronic occupation function $f_n(r, k, t)$ becomes an explicit function of momentum, space, and time whose total derivative versus time vanishes because the total number of particles is conserved along the trajectories of the phase space:

$$\begin{aligned} \frac{df_{n,k}}{dt} &= \frac{\partial f_{n,k}}{\partial t} + \nabla_k f_{n,k} \frac{d\mathbf{k}}{dt} + \nabla_r f_{n,k} \frac{d\mathbf{r}}{dt} \\ &\equiv \frac{\partial f_{n,k}}{\partial t} + \frac{1}{\hbar} \nabla_k f_{n,k} \cdot \mathbf{F} + \nabla_r f_{n,k} \cdot \mathbf{v}_k = 0. \end{aligned} \quad (2.2)$$

In the following, for the sake of simplicity, we neither consider the application of any magnetic field nor the occurrence of any temperature and carrier concentration gradients [this last point eliminates the space gradient in Eq. (2.2)]. Separating the forces acting on electrons into the applied force $\mathbf{F}_A = e\mathbf{E}$ and internal forces due to collision events, we obtain

$$\begin{aligned} \frac{\partial f_{n,k}}{\partial t} &= -\frac{1}{\hbar} \nabla_k f_{n,k} \cdot \mathbf{F}_A - \frac{1}{\hbar} \nabla_k f_{n,k} \cdot \mathbf{F}_{\text{int}} \\ &\equiv -\frac{1}{\hbar} \nabla_k f_{n,k} \cdot \mathbf{F}_A + \left(\frac{\partial f_{n,k}}{\partial t} \right)_{\text{coll}}. \end{aligned} \quad (2.3)$$

When the stationary state is reached, the explicit variation of f with time vanishes. For weak applied fields, we write

$$f_n(r, k, t) = f_0(E_{n,k}) + \delta f_{n,k}. \quad (2.4)$$

With such a notation, neglecting second-order terms in fields, Eq. (2.3) becomes

$$\left(\frac{\partial f_{n,k}}{\partial t} \right)_{\text{coll}} \equiv \frac{1}{\hbar} \nabla_k f_0(E_{n,k}) \cdot \mathbf{F}_A \equiv \frac{\partial f_0(E_{n,k})}{\partial E_{n,k}} \mathbf{F}_A \cdot \mathbf{v}_{n,k}. \quad (2.5)$$

The collision term is statistically described, using the transition probability $W_{n,n'}(k, k')$ per unit time due to collision events between the various $E_n(k)$ energy states. For a multisubband system it gives

$$\left(\frac{\partial f_{n,k}}{\partial t}\right)_{\text{coll}} = \sum_{n',k'} [W_{n',n}(k',k)f_{n',k'}(1-f_{n,k}) - W_{n,n'}(k,k')f_{n,k}(1-f_{n',k'})]. \quad (2.6)$$

In Eq. (2.6), the first term of the right side represents the effect of transition from a k' state belonging to subband n' toward a k state belonging to subband n which leads to an increase of $\partial f_{n,k}/\partial t$, while the second term corresponds to a transition, from a (n, k) state towards any other (n', k') state which leads to a decrease of $\partial f_{n,k}/\partial t$. Both contributions are obviously weighted by the occupation rate f of the initial state and non occupation rate $(1-f)$ of the final state. Introducing Eq. (2.4) into Eq. (2.6), we obtain at first order (i.e., neglecting δf^2 terms)

$$\begin{aligned} \left(\frac{\partial f_{n,k}}{\partial t}\right)_{\text{coll}} &= \sum_{n',k'} \{W_{n',n}(k',k)[1-f_0(E_{n,k})] \\ &+ W_{n,n'}(k,k')f_0(E_{n,k})\} \delta f_{n',k'} \\ &- \delta f_{n,k} \sum_{n',k'} \{W_{n',n}(k',k)f_0(E_{n',k'}) \\ &+ W_{n,n'}(k,k')[1-f_0(E_{n',k'})]\}. \end{aligned} \quad (2.7)$$

Let us define the ‘‘quantum lifetime’’

$$\frac{1}{\tau_{0,n}(\mathbf{k})} = \sum_{n',k'} W_{n',n}(k',k)f_0(E_{n',k'}) + W_{n,n'}(k,k') \times [1-f_0(E_{n',k'})] \quad (2.8)$$

and introduce the notation

$$G_{n,n'}(k,k') = W_{n',n}(k',k)[1-f_0(E_{n,k})] + W_{n,n'}(k,k')f_0(E_{n,k}). \quad (2.9)$$

With these definitions and using Eq. (2.5), we finally obtain the so-called linearized Boltzmann equation

$$\begin{aligned} \delta f_{n,k} &= -\frac{\partial f_0(E_{n,k})}{\partial E_{n,k}} (\mathbf{v}_{n,k} \cdot \mathbf{F}_A) \tau_{0,n}(\mathbf{k}) \\ &\times \left(1 - \sum_{n',k'} G_{n,n'}(k,k') \frac{\delta f_{n',k'}}{\frac{\partial f_0(E_{n,k})}{\partial E_{n,k}} (\mathbf{v}_{n,k} \cdot \mathbf{F}_A)} \right). \end{aligned} \quad (2.10)$$

Expression (2.10) implies that $\delta f_{n,k}$ may also be written in the form

$$\delta f_{n,k} = -\frac{\partial f_0(E_{n,k})}{\partial E_{n,k}} (\mathbf{v}_{n,k} \cdot \mathbf{F}_A) \tau_n(k). \quad (2.11)$$

Introducing this form in the right term of expression (2.10) unambiguously demonstrates that a relaxation time $\tau_n(\mathbf{k})$ may be defined in any circumstances (anisotropic and inelastic scattering mechanisms):

$$\begin{aligned} \tau_n(k) &= \tau_{0,n}(k) \left(1 + \sum_{n',k'} G_{n,n'}(k,k') \right. \\ &\times \left. \frac{f_0(E_{n',k'})[1-f_0(E_{n',k'})](\mathbf{k}' \cdot \mathbf{F}_A)}{f_0(E_{n,k})[1-f_0(E_{n,k})](\mathbf{k} \cdot \mathbf{F}_A)} \tau_{n'}(k') \right), \end{aligned} \quad (2.12)$$

where we have made use of the identity $\partial f_0/\partial \varepsilon = -f_0(\varepsilon)[1-f_0(\varepsilon)]/KT$.

The functions $G_{n,n'}(k,k')$ depend on the simultaneous occurrence of different elastic and inelastic scattering mechanisms. For elastic mechanisms it is obvious that $W_{n,n'}(k,k') = W_{n',n}(k',k)$ [as shown by the Fermi golden rule expression (2.18)]. If we restrict the derivation to the case of inelastic scattering processes characterized by only one frequency ω (optical phonons, for instance), in the presence of various elastic (or quasielastic) processes (impurities, acoustic phonons) characterized by the subscript β , expressions (2.8) and (2.9) may be also written in the form

$$\begin{aligned} \frac{1}{\tau_{0,n}(\mathbf{k})} &= \sum_{n',k'} W_{n',n}^{\text{inel}}(k',k)f_0(E_{n',k'}) + W_{n,n}^{\text{inel}}(k,k') \\ &\times [1-f_0(E_{n',k'})] + \sum_{\beta, n', k'} W_{n,n'}^{\beta, \text{elas}}(k,k') \\ &\equiv \frac{1}{\tau_{0,n}^{\text{inel}}(\mathbf{k})} + \sum_{n', \beta, k'} W_{n,n'}^{\beta, \text{elas}}(k,k') \end{aligned} \quad (2.13)$$

and

$$\begin{aligned} G_{n,n'}(k,k') &= W_{n',n}^{\text{inel}}(k',k)[1-f_0(E_{n,k})] \\ &+ W_{n,n}^{\text{inel}}(k,k')f_0(E_{n,k}) + \sum_{\beta} W_{n,n}^{\beta, \text{elas}}(k,k'). \end{aligned} \quad (2.14)$$

Inserting Eq. (2.14) into Eq. (2.12) and restricting the present derivation to the case of isotropic scattering mechanisms for which $\tau(\mathbf{k}) = \tau(k) = \tau(\varepsilon_k)$, we obtain

$$\begin{aligned} \tau_n(\varepsilon_k) &= \tau_{0,n}^{\text{total}}(\varepsilon_k) \left[1 + \sum_{n',k'} \left(G_{n,n'}^{\text{inel}}(k,k') \right. \right. \\ &\times \left. \frac{f_0(E_{n',k'})[1-f_0(E_{n',k'})]}{f_0(E_{n,k})[1-f_0(E_{n,k})]} \right. \\ &\left. \left. + \sum_{\beta} W_{n,n'}^{\beta, \text{elas}}(k,k')[1-\delta_{nn'}] \right) \cos(\theta) \tau_{n'}(\varepsilon_{k'}) \right], \end{aligned} \quad (2.15)$$

where θ is the angle between k and k' and where we have defined

$$\frac{1}{\tau_{0,n}^{\text{total}}(\varepsilon_k)} = \frac{1}{\tau_{0,n}^{\text{inel}}(\varepsilon_k)} + \sum_{\beta} \frac{1}{\tau_n^{\beta, \text{elas}}(\varepsilon_k)} + \sum_{\substack{n' \neq n \\ \beta, k'}} W_{n,n'}^{\beta, \text{elas}}(k,k'), \quad (2.16)$$

with

$$\frac{1}{\tau_n^{\beta, \text{elas}}(\varepsilon_k)} = \sum_{k'} W_{n,n}^{\beta, \text{elas}}(k, k') [1 - \cos(\theta)]. \quad (2.17)$$

Note that expression (2.17) corresponds to the classical relaxation time defined for elastic and isotropic scattering mechanisms within a single band.

The various transition probabilities per unit time are given by the Fermi golden rule

$$W_{n,n'}^{\pm}(k, k') = \frac{2\pi}{\hbar} |\langle n, k | \hat{V}(\pm\omega) | n', k' \rangle|^2 \times \delta(E_{n', k'} - E_{n, k} \pm \hbar\omega). \quad (2.18)$$

The \pm symbols indicate the possibility of emission or absorption processes. Introducing the notation $\langle n, k | \hat{V}(\pm\omega) | n', k' \rangle = V_{n,n'}^{\pm}(q)$ with $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, the various $G_{n,n'}^{\text{inel}}(k, k')$ functions may also be written in the form

$$G_{n,n'}^{\text{inel}}(k, k') = \frac{2\pi}{\hbar} |V_{n,n'}^+(q)|^2 \{ \delta(E_{n,k} - E_{n',k'} + \hbar\omega) [1 - f_0(E_{n,k})] + \delta(E_{n',k'} - E_{n,k} + \hbar\omega) f_0(E_{n,k}) \} + \frac{2\pi}{\hbar} |V_{n,n'}^-(q)|^2 \{ \delta(E_{n,k} - E_{n',k'} - \hbar\omega) [1 - f_0(E_{n,k})] + \delta(E_{n',k'} - E_{n,k} - \hbar\omega) f_0(E_{n,k}) \}, \quad (2.19)$$

where we have separated the scattering mechanisms corresponding either to emission (+) or absorption (−) processes. Inserting Eq. (2.19) into Eq. (2.15) and replacing the summation over k' by an integral, we obtain [for a two-dimensional (2D) system]

$$\tau_n(\varepsilon_k) = \tau_{0,n}^{\text{total}}(\varepsilon_k) + \sum_{n'} M^{n,n'}(\varepsilon_k) \tau_{n'}(\varepsilon_k - [\hbar\omega + E_{n'} - E_n]) + \sum_{n'} P^{n,n'}(\varepsilon_k) \tau_{n'}(\varepsilon_k + [\hbar\omega + E_n - E_{n'}]) + \sum_{n' \neq n} B^{n,n'}(\varepsilon_k) \tau_{n'}(\varepsilon_k - E_{n'} + E_n), \quad (2.20)$$

with $M^{n,n'}(\varepsilon_k) = 0$ if $\varepsilon_k < \hbar\omega + E_{n'} - E_n$; otherwise,

$$M^{n,n'}(\varepsilon_k) = \tau_n^{\text{total}}(\varepsilon_k) \frac{m^*}{2\pi\hbar^3} \int_0^{2\pi} \left\{ \frac{|V_{n,n'}^+(q_1)|^2}{1 - f_0(E_{n,k})} + \frac{|V_{n,n'}^-(q_1)|^2}{f_0(E_{n,k})} \right\} \times \cdots \times f_0(E_{n,k} - \hbar\omega) \times [1 - f_0(E_{n,k} - \hbar\omega)] \times \sqrt{1 - \frac{\hbar\omega + E_{n'} - E_n}{\varepsilon_k} \cos\theta} d\theta, \quad (2.21a)$$

with

$$q_1 = \sqrt{2k^2 \left(1 - \frac{\hbar\omega + E_{n'} - E_n}{2\varepsilon_k} - \sqrt{1 - \frac{\hbar\omega + E_{n'} - E_n}{\varepsilon_k} \cos(\theta)} \right)}. \quad (2.21b)$$

$P^{n,n'}(\varepsilon_k) = 0$ if $\varepsilon_k < E_{n'} - E_n - \hbar\omega$; otherwise,

$$P^{n,n'}(\varepsilon_k) = \tau_n^{\text{total}}(\varepsilon_k) \frac{m^*}{2\pi\hbar^3} \int_0^{2\pi} \left\{ \frac{|V_{n,n'}^+(q_2)|^2}{f_0(E_{n,k})} + \frac{|V_{n,n'}^-(q_2)|^2}{1 - f_0(E_{n,k})} \right\} \times \cdots \times f_0(E_{n,k} + \hbar\omega) [1 - f_0(E_{n,k} + \hbar\omega)] \times \sqrt{1 + \frac{\hbar\omega + E_n - E_{n'}}{\varepsilon_k} \cos(\theta)} d\theta, \quad (2.22a)$$

with

$$q_2 = \sqrt{2k^2 \left(1 + \frac{\hbar\omega + E_n - E_{n'}}{2\varepsilon_k} - \sqrt{1 + \frac{\hbar\omega + E_n - E_{n'}}{\varepsilon_k} \cos(\theta)} \right)}. \quad (2.22b)$$

and where $B^{n,n'}(\varepsilon_k) = 0$ if $\varepsilon_k < E_{n'} - E_n$; otherwise,

$$B^{n,n'}(\varepsilon_k) = \tau_n^{\text{total}}(\varepsilon_k) \frac{m^*}{2\pi\hbar^3} \int_0^{2\pi} \sum_{\beta} |V_{n,n'}^{\beta}(q)|^2 \times \sqrt{1 - \frac{E_{n'} - E_n}{\varepsilon_k} \cos\theta} d\theta, \quad (2.23a)$$

with

$$q = \sqrt{2k^2 \left(1 + \frac{E_n - E_{n'}}{2\varepsilon_k} - \sqrt{1 + \frac{E_n - E_{n'}}{\varepsilon_k} \cos(\theta)} \right)}. \quad (2.23b)$$

The set of equations (2.20) are an extension of the linear-

ized Boltzmann equation obtained, for instance, in Refs. 9 and 10, but generalized in the case (i) of a multisubband system and (ii) where elastic and inelastic scattering centers act simultaneously. Because of the presence of intersubband contributions, Eqs. (2.20) do not have any more simple solutions, even in a pure numerical form, although the contribution of such intersubband transitions does not bring any particular difficulty in the calculation of $\tau_{0,n}^{\text{total}}(\varepsilon_k)$.

B. Numerical solutions

Numerical solutions may, however, be obtained using the following remark: the various matrix elements $V_{n,n'}$, corresponding to intersubband transitions are weak when compared to matrix elements corresponding to intrasubband transitions. Thus, in a first step, approximate solutions $\tau_n^{(0)}(\varepsilon_k)$ of Eqs. (2.20) are calculated, introducing the intersubband contributions in the calculation of $\tau_{0,n}^{\text{total}}(\varepsilon_k)$, but neglecting them in Eq. (2.20), which, thus, transforms into a set of independent equations for each subband n :

$$\tau_n^{(0)}(\varepsilon_k) = \tau_{0,n}^{\text{total}}(\varepsilon_k) + M^{n,n}(\varepsilon_{n,k})\tau_n^{(0)}(\varepsilon_k - \hbar\omega) + P^{n,n}(\varepsilon_{n,k})\tau_n^{(0)}(\varepsilon_k + \hbar\omega). \quad (2.24)$$

Solutions of Eq. (2.24) can be found using different methods (variational methods,¹¹⁻¹⁴ iteration methods,¹⁵ etc.). In the following, we use a method similar to that recently used by Anderson *et al.*^{9,10} (the so-called ladder technique) and

which is based on the following remark: Any value of the kinetic energy may always be written in the form $\varepsilon_k = j\hbar\omega + \delta\varepsilon$ ($j=0, 1, 2, 3\dots$ being an integer). Writing

$$\tau_n^{(0)}(\varepsilon_k) = \tau_n^{(0)}(j\hbar\omega + \delta\varepsilon) = \tau_{n,j}^{(0)}(\delta\varepsilon) \quad (2.25)$$

and introducing similar notation for the functions M and P , Eq. (2.24) gives rise for each subband n to an infinite set of linear equations

$$-M_j^{n,n}\tau_{n,j-1}^{(0)}(\delta\varepsilon) + \tau_{n,j}^{(0)}(\delta\varepsilon) - P_j^{n,n}(\delta\varepsilon)\tau_{n,j+1}^{(0)}(\delta\varepsilon) = \tau_{0,n,j}^{\text{total}}(\delta\varepsilon), \quad (2.26)$$

with $M_0^{n,n}=0$. Following Refs. 9, 10, and 16, we assume that at large energies $\varepsilon = N\hbar\omega_0 + \delta\varepsilon$, we may approximate $\tau_n^{(0)}(\varepsilon) \cong \tau_n^{(0)}(\varepsilon + \hbar\omega) \cong \tau_n^{(0)}(\varepsilon - \hbar\omega)$. This leads to

$$\tau_{n,N}^{(0)}(\delta\varepsilon) \cong \frac{\tau_{0,n,N}^{\text{total}}(\delta\varepsilon)}{1 - M_N^{n,n} - P_N^{n,n}}. \quad (2.27)$$

This also allows the infinite set of linear equations (2.26) to be truncated for $j=N$ and to be transformed into a finite linear set of equations of order N . It can be put in a matrix form (as, the example, given above for $N=10$) that can be very easily numerically solved for any $\delta\varepsilon$ value even for large values of N :

$$\begin{pmatrix} 1 & -p_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -m_2 & 1 & -p_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -m_3 & 1 & -p_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -m_4 & 1 & -p_4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -m_5 & 1 & -p_5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -m_6 & 1 & -p_6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -m_7 & 1 & -p_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -m_8 & 1 & -p_8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -m_9 & 1 & -p_9 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 - m_{10} - P_{10} \end{pmatrix} \times \begin{pmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \tau_5 \\ \tau_6 \\ \tau_7 \\ \tau_8 \\ \tau_9 \\ \tau_{10} \end{pmatrix} = \begin{pmatrix} \tau_{0,1} \\ \tau_{0,2} \\ \tau_{0,3} \\ \tau_{0,4} \\ \tau_{0,5} \\ \tau_{0,6} \\ \tau_{0,7} \\ \tau_{0,8} \\ \tau_{0,9} \\ \tau_{0,10} \end{pmatrix}. \quad (2.28)$$

This procedure requires a very low computation demand and allows the determination of the relaxation time $\tau_n^{(0)}(\varepsilon_k)$ in the whole energy range of interest.

Once the zero-order values $\tau_n^{(0)}(\varepsilon_k)$ have been determined in the whole energy range of interest, we come back to Eqs. (2.20) and write

$$\tau_n(\varepsilon_k) = \tau_n^{(0)}(\varepsilon_k) + \delta\tau_n(\varepsilon_k). \quad (2.29)$$

Introducing this form into Eqs. (2.20), it is straightforward to see that the $\delta\tau_n(\varepsilon_k)$ are solutions of the following set of equations:

$$\begin{aligned}
 \delta\tau_n(\varepsilon_k) = & g_n(\varepsilon_k) + \sum_{n' \neq n} M^{n,n'}(\varepsilon_{n,k}) \delta\tau_{n'}(\varepsilon_k - [\hbar\omega + E_{n'} \\
 & - E_n]) + \sum_{n' \neq n} P^{n,n'}(\varepsilon_{n,k}) \delta\tau_{n'}(\varepsilon_k + [\hbar\omega + E_n \\
 & - E_{n'}]) + \sum_{n' \neq n} B^{n,n'}(\varepsilon_{n,k}) \delta\tau_{n'}(\varepsilon_k + [E_n - E_{n'}]),
 \end{aligned} \quad (2.30)$$

where we have introduced the fully numerically known functions

$$\begin{aligned}
 g_n(\varepsilon_k) = & \sum_{n' \neq n} M^{n,n'}(\varepsilon_{n,k}) \tau_{n'}^{(0)}(\varepsilon_k - [\hbar\omega + E_{n'} - E_n]) \\
 & + \sum_{n' \neq n} P^{n,n'}(\varepsilon_{n,k}) \tau_{n'}^{(0)}(\varepsilon_k + [\hbar\omega + E_n - E_{n'}]) \\
 & + \sum_{n' \neq n} B^{n,n'}(\varepsilon_{n,k}) \tau_{n'}^{(0)}(\varepsilon_k + E_n - E_{n'}). \quad (2.31)
 \end{aligned}$$

Since the functions $M^{n,n'} \delta\tau_n$, $P^{n,n'} \delta\tau_n$, and $B^{n,n'} \delta\tau_n$ get very weak values compared to that of g_n , Eq. (2.30) can then be solved by iteration starting from

$$\delta\tau_n^{(1)}(\varepsilon_k) = g_n(\varepsilon_k) \quad (2.32a)$$

and iteratively calculating

$$\begin{aligned}
 \delta\tau_n^{(J)}(\varepsilon_k) = & g_n(\varepsilon_k) + \sum_{n' \neq n} M^{n,n'}(\varepsilon_{n,k}) \delta\tau_{n'}^{(J-1)}(\varepsilon_k - [\hbar\omega \\
 & + E_{n'} - E_n]) + \sum_{n' \neq n} P^{n,n'}(\varepsilon_{n,k}) \delta\tau_{n'}^{(J-1)}(\varepsilon_k \\
 & + [\hbar\omega + E_n - E_{n'}]) + \sum_{n' \neq n} B^{n,n'}(\varepsilon_{n,k}) \delta\tau_{n'}^{(J-1)} \\
 & \times (\varepsilon_k + [E_n - E_{n'}]). \quad (2.32b)
 \end{aligned}$$

Numerical results show that this procedure converges very quickly. We found that five to ten iterations were sufficient to get the final exact numerical result.

As an example, we have calculated the carrier mobility in the case of an AlGaIn/GaN quantum well containing a total carrier density of $4 \times 10^{12} \text{ cm}^{-2}$ at 300 K and four subbands whose two first are noticeably occupied by electrons (Table I). The various energy states and their associated wave functions (needed for the determination of the transition matrix elements) have been determined using the numerical procedure described in the following paper of this series. Figures 1 and 2, respectively, show the relaxation times associated with the four subbands. Numerical results have been obtained considering a combination of scattering mechanisms associated with phonons (acoustic deformation potential and piezoelectric potential, polar optical phonons) combined with ionized impurity scattering (10^{18} cm^{-3}) and dislocations ($5 \times 10^9 \text{ cm}^{-2}$). Figure 1 corresponds to the case where the intersubband transitions are neglected and which leads to a

TABLE I. Energy levels calculated at 300 K for an AlGaIn/GaN triangular quantum well of depth 0.7 meV.

Energy level (meV)	91.66 meV	200.5 meV	386	622
Carrier density (cm^{-2})	3.86×10^{12}	1.4×10^{11}	1.1×10^8	~ 0

mobility equal to $4133 \text{ cm}^2/\text{V s}$. It exhibits discontinuities at energy values equal to multiples of the optical phonon energy $\hbar\omega$. Figure 2 is obtained including intersubband transitions, which leads to a mobility equal to $3830 \text{ cm}^2/\text{V s}$. This last figure also exhibits supplementary discontinuities occurring at energy values corresponding to $E_{n'} - E_n \pm \hbar\omega$. The difference between the mobility values demonstrates that intersubband transitions lead to noticeable effects on the free carrier mobility and cannot be neglected in the study of the free carrier mobility in a multiply occupied subband system.

III. MULTISUBBAND 2D DIELECTRIC FUNCTION

A. General expression

The matrix elements needed for the calculation of the collision time correspond to the screened potential: sum of the unscreened potential matrix elements (noted by the symbol “ext”) and of the matrix elements of the potential induced by the dielectric response of the electronic system (noted by the symbol “ind”). Thus,

$$V_{n,n'}^{\pm\omega_0,\text{tot}}(q) = V_{n,n'}^{\pm\omega_0,\text{ext}}(q) + V_{n,n'}^{\pm\omega_0,\text{ind}}(q). \quad (3.1)$$

These matrix elements are calculated between the quantum well wave functions given by

$$\langle r | n, k \rangle = \varphi_n(\mathbf{r}) = \varphi_n(\boldsymbol{\rho}, z) = \frac{1}{\sqrt{S}} e^{i\mathbf{k} \cdot \boldsymbol{\rho}} Z_n(z), \quad (3.2)$$

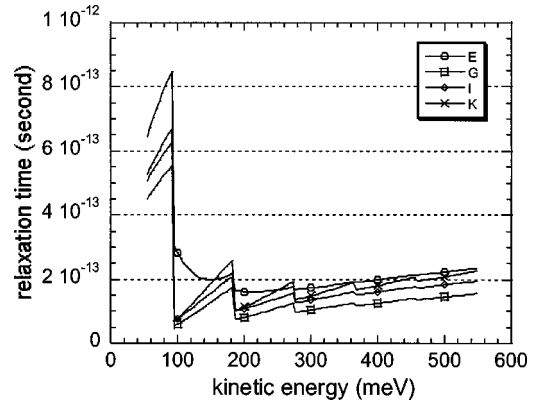


FIG. 1. Relaxation time calculated at 300 K for each subband of an AlGaIn/GaN triangular quantum well, neglecting intersubband transitions. The corresponding free carrier mobility taking into account acoustic and optical phonon scattering, ionized impurities, and dislocations is found equal to $4133 \text{ cm}^2/\text{V s}$. Curves E, G, I, and K, respectively, represent the relaxation time associated with subbands 1, 2, 3, and 4.

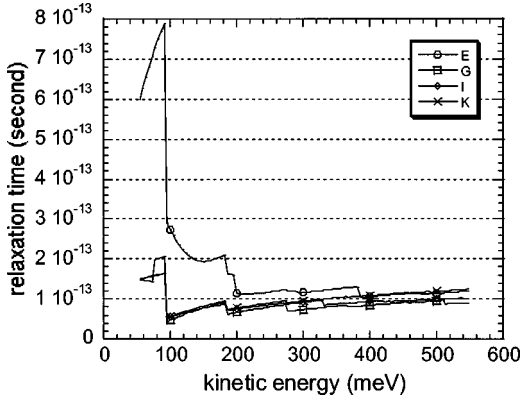


FIG. 2. Relaxation time calculated at 300 K for each subband of an AlGaIn/GaN triangular quantum well, including intersubband transitions. The corresponding free carrier mobility taking into account acoustic and optical phonon scattering, ionized impurities, and dislocations is found equal to $3830 \text{ cm}^2/\text{V s}$. Curves E, G, I, and K, respectively, represent the relaxation time associated with subbands 1, 2, 3, and 4.

where $Z_n(z)$ is the envelop function associated with subband n . They are given by

$$\begin{aligned} \langle n, k | e V^{\text{tot}}(r, \omega) | n', k' \rangle \\ = \delta_{k', k+q} \int e V^{\text{tot}}(q, z, \omega) Z_n^*(z) Z_{n'}(z) dz \\ = \delta_{k', k+q} M_{n, n'}^{\text{tot}}(q, \omega) \end{aligned} \quad (3.3)$$

and similar expressions for $M_{n, n'}^{\text{ext}}(q, \pm \omega_0)$ and $M_{n, n'}^{\text{ind}}(q, \pm \omega_0)$. The induced potential is connected to the induced charge through Poisson's equation

$$\begin{aligned} \Delta V^{\text{ind}}(\mathbf{r}, \omega) = - \frac{n^{\text{ind}}(\mathbf{r}, \omega)}{\epsilon_0} \rightarrow \frac{d^2 V^{\text{ind}}(q, z, \omega)}{dz^2} \\ = q^2 V^{\text{ind}}(q, z, \omega) - \frac{n^{\text{ind}}(\mathbf{q}, z, \omega)}{\epsilon_0}. \end{aligned} \quad (3.4)$$

Making use of the Green function technique, the solution of Eq. (3.4) may be written in the form

$$V^{\text{ind}}(\mathbf{q}, z, \omega) = \int_{-\infty}^{\infty} G(\mathbf{q}, z, z') n^{\text{ind}}(\mathbf{q}, z', \omega) dz', \quad (3.5)$$

where the Green function $G(q, z, z')$ is the solution of

$$\frac{d^2 G(q, z, z')}{dz^2} = q^2 G(q, z, z') - \frac{\delta(z - z')}{\epsilon_0}. \quad (3.6)$$

The induced matrix elements are then given by

$$\begin{aligned} M_{n, n'}^{\text{ind}}(q, \pm \omega_0) = \delta_{k', k \mp q} \int G(q, z, z') n^{\text{ind}}(q, z', \\ \pm \omega_0) Z_n^*(z) Z_{n'}(z) dz dz'. \end{aligned} \quad (3.7)$$

The induced charge contribution is calculated using the density operator $\hat{\rho}_0 = \sum_{n, k} |n, k\rangle f_0(\epsilon_{n, k}) \langle n, k|$. When any perturbation $e V^{\text{tot}}(r, \omega)$ is applied to the electronic system, this op-

erator experiences a variation $\delta \hat{\rho}$ whose matrix elements between two electronic states are given by^{17,18}

$$\begin{aligned} \delta \rho_{n, k, n', k'} \\ = e \frac{f_0(\epsilon_{n', k'}) - f_0(\epsilon_{n, k})}{\epsilon_{n', k'} - \epsilon_{n, k} - \hbar \omega + i \hbar \alpha} \langle n, k | V^{\text{tot}}(r, \omega) | n', k' \rangle, \end{aligned} \quad (3.8)$$

where α is an infinitely small positive number accounting for the adiabatic switch on of the perturbation. In the Schrödinger representation, the electron density may be represented by the operator $\hat{n}(r) = e \delta(r - r_e)$, where r_e stands for the electron coordinate. The induced charge is given by

$$\begin{aligned} n^{\text{ind}}(r, \omega) = \text{Tr} \{ \delta \hat{\rho} \cdot \hat{n}(r) \} = e \sum_{n, k, n', k'} \delta \rho_{n, k, n', k'}(\omega) \\ \times \langle n', k' | \delta(r - r_e) | n, k \rangle. \end{aligned} \quad (3.9)$$

Introducing Eq. (3.8) into Eq. (3.9), the induced charge is therefore

$$\begin{aligned} n^{\text{ind}}(q, z, \pm \omega_0) \\ = e^2 \sum_{m, m'} \sum_k \frac{f(\epsilon_{m', k \mp q}) - f(k)}{\epsilon_{m', k \mp q} - \epsilon_{m, k} \mp \hbar \omega_0 + i \hbar \alpha} \\ \times M_{m, m'}^{\text{tot}}(q, \pm \omega_0) Z_m^*(z) Z_m(z). \end{aligned} \quad (3.10)$$

Introducing Eq. (3.10) into Eq. (3.7), we straightforwardly obtain

$$M_{n, n'}^{\text{ind}}(q, \pm \omega_0) = \sum_{m, m'} \chi_{n, n'}^{m, m'}(q, \omega_0) M_{m, m'}^{\text{tot}}(q, \pm \omega_0),$$

with

$$\begin{aligned} \chi_{n, n'}^{m, m'}(q, \omega_0) \\ = e^2 \sum_k \frac{f(\epsilon_{m', k \mp q}) - f(\epsilon_{m, k})}{\epsilon_{m', k \mp q} - \epsilon_{m, k} \mp \hbar \omega_0 + i \hbar \alpha} \int G(q, z, z') \\ \times Z_n^*(z) Z_{n'}(z) Z_m^*(z') Z_m(z') dz dz'. \end{aligned} \quad (3.11)$$

Adding to both sides of Eq. (3.11) the external matrix element $M_{n, n'}^{\text{ext}}(q, \pm \omega_0)$, we obtain

$$\begin{aligned} M_{n, n'}^{\text{tot}}(q, \pm \omega_0) = M_{n, n'}^{\text{ext}}(q, \pm \omega_0) + \sum_{m, m'} \chi_{n, n'}^{m, m'}(q, \pm \omega_0) \\ \times M_{m, m'}^{\text{tot}}(q, \pm \omega_0), \end{aligned} \quad (3.12)$$

which may as well be written

$$\sum_{m, m'} \epsilon_{n, n'}^{m, m'}(q, \pm \omega) M_{m, m'}^{\text{tot}}(q, \pm \omega) = M_{n, n'}^{\text{ext}}(q, \pm \omega), \quad (3.13)$$

where we have introduced a tensor of dielectric functions whose components are given by

$$\varepsilon_{n,n'}^{m,m'}(q, \pm \omega_0) = \delta_{n,m} \delta_{n',m'} - \chi_{n,n'}^{m,m'}(q, \pm \omega_0), \quad (3.14)$$

with

$$\chi_{n,n'}^{m,m'}(q, \pm \omega_0) = I_{n,n',m,m'}(q) \zeta_{m,m'}(q, \pm \omega_0), \quad (3.15)$$

where

$$\begin{aligned} I_{n,n',m,m'}(q) \\ = \int G(q, z, z') Z_n^*(z) Z_{n'}(z) Z_m^*(z') Z_{m'}(z') dz dz' \end{aligned} \quad (3.16a)$$

and

$$\zeta_{m,m'}(q, \pm \omega) = e^2 \sum_k \frac{f(\varepsilon_{m',k\mp q}) - f(\varepsilon_{m,k})}{\varepsilon_{m',k\mp q} - \varepsilon_{m,k} \mp \hbar \omega + i \hbar \alpha}. \quad (3.16b)$$

Expression (3.13) shows that the screened matrix elements acting on the conductivity of a given subband are solutions of a linear set of equations and will therefore depend on the matrix elements of the external (unscreened) potential calculated between all other subband wave functions.

B. Approximate expressions of the dielectric function tensor

The determination of the various components of the dielectric function tensor depends on our capability of estimating the $I_{n,n',m,m'}(q)$ and $\zeta_{m,m'}(q, \omega)$ functions. The $I_{n,n',m,m'}(q)$ function depends on the heterostructure geometry and on its bound states wave functions. Let us, for instance, consider the particular case of AlGaIn/GaN quantum wells whose heterostructures are made of a GaN substrate which constitutes quite a semi-infinite medium of relative permittivity ε_2 and an AlGaIn top layer with a finite thickness d and permittivity ε_1 . In general, the quantum well will bind energy states whose wave function will be confined to the GaN region. Thus a good approximation consists in considering that the quantum well is indeed located between two semi-infinite media. Moreover, in this particular AlGaIn/GaN case, the permittivities of the two media are very near so that a (strongly) simplifying assumption is to put $\varepsilon_1 = \varepsilon_2 = \varepsilon_L$. In such a case, an appropriate expression for the Green function is

$$G(q, z, z') = \frac{1}{2q\varepsilon_L} e^{-q|z-z'|}. \quad (3.17)$$

The full determination of $I_{n,n',m,m'}(q)$ depends also on the actual wave functions of the quantum well. These functions have to be determined using an alternate and iterative solution of the Schrödinger and Poisson equations. Although this can be formally done numerically (as shown in paper II in this series), such a procedure will lead to lengthy and inextricable calculations. Instead, we can make the crude but realistic approximation that most of the scattering potentials are long range and therefore described by Fourier transforms that are only preeminent for small q values. Moreover, the

wave functions are localized and vanish for large z values. These two combined arguments allow us to approximate

$$\begin{aligned} I_{n,n',m,m'}(q) \\ = \frac{1}{2q\varepsilon_L} \int e^{-q|z-z'|} Z_n^*(z) \\ \times Z_{n'}(z) Z_m^*(z') Z_{m'}(z') dz dz' \\ \cong \frac{1}{2q\varepsilon_L} \int Z_n^*(z) Z_{n'}(z) Z_m^*(z') Z_{m'}(z') dz dz' \\ = \frac{\delta_{n,n'} \delta_{m,m'}}{2\varepsilon_L q}. \end{aligned} \quad (3.18)$$

Then the above result suppresses the necessity to calculate the $\zeta_{m,m'}(q, \omega)$ for m different from m' . Restricting the following derivation to the case of the static dielectric response, we just have to calculate $\zeta_{m,m}(q, 0)$, which in the ‘‘small- q ’’ approximation gives

$$\begin{aligned} \zeta_{m,m}(q, 0) = e^2 \sum_k \frac{f(\varepsilon_{m,k\mp q}) - f(\varepsilon_{m,k})}{\varepsilon_{m,k\mp q} - \varepsilon_{m,k}} \\ = e^2 \sum_k \left(\frac{\partial f}{\partial \varepsilon} \right)_{m,k} = - \frac{m^* e^2}{\pi \hbar^2} f(\varepsilon_m). \end{aligned} \quad (3.19)$$

Thus

$$\varepsilon_{n,n'}^{m,m'}(q, 0) = \delta_{n,m} \delta_{n',m'} + \frac{k_{sc,m}}{q} \delta_{n,n'} \delta_{m,m'}, \quad (3.20)$$

where we have introduced a set of screening wave vectors $k_{so,m}$ given by

$$k_{sc,m} = \frac{m^* e^2 f(\varepsilon_m)}{2\pi \hbar^2 \varepsilon_L}. \quad (3.21)$$

Introducing Eq. (3.20) into Eq. (3.12), we straightforwardly obtain

$$M_{n,n}^{\text{tot}} = \frac{M_{n,n}^{\text{ext}} + \sum_m (M_{n,n}^{\text{ext}} - M_{m,m}^{\text{ext}}) \frac{k_{sc,m}}{q}}{1 + \frac{k_{2D}}{q}}, \quad (3.22)$$

where we have defined $k_{2D} = \sum_m k_{sc,m}$.

Note that, within our approximation, intersubband matrix elements remain unscreened. On the contrary, expression (3.22) shows that the actual potential which acts on the carrier mobility in one given subband depends on the participation to the full screening of all the occupied subbands. A comparison may be made with the case of 3D homogeneous systems where the dielectric tensor would become, in the Debye-Hückel approximation,

$$\varepsilon_{n,n'}^{m,m'}(q, 0) = \delta_{n,m} \delta_{n',m'} + \frac{k_{DH,m}^2}{q^2} \delta_{n,n'} \delta_{m,m'}, \quad (3.23)$$

with $k_{DH,m}^2 = n_m e^2 / (\varepsilon_0 \varepsilon_L K T)$. In the case where the conductivity would simultaneously result from electrons in the conduction band and holes in the valence bands, then, the

screened scattering matrix elements would be given by expressions equivalent Eq. (3.22). However, the external (unscreened) elements are, in this 3D case, calculated between pure plane waves in both the conduction and valence bands and are therefore identical so that the screened matrix elements are both identical for all bands and reduce to the usual expression

$$M_{c,c}^{\text{tot}} = M_{v,v}^{\text{tot}} = \frac{M^{\text{ext}}}{1 + \frac{k_{\text{DH,G}}^2}{q^2}}, \quad (3.24)$$

with $k_{\text{DH,G}}^2 = (n+p)e^2/(\epsilon_0\epsilon_LKT)$. This comparison points out the fact that, in the case of different 2D subbands, screening effects, as usual, issue from all the electrons present in the various subbands of the structure, but the apparent complexity of the numerators entering Eq. (3.22) results from the fact that all of them do not have the same z localization since they belong to different envelope functions.

IV. CONCLUSION

The study of the low-field conductivity in AlGaIn/GaN quantum wells necessitates the possibility of describing optical phonon scattering combined with other elastic scattering mechanisms. To solve this problem, numerical techniques have been developed to find solutions of the linearized Boltzmann equation generalized to the case of a multisubband system. Moreover, we could derive approximate expressions of the screened potentials acting on the various occupied subbands of the quantum well. In paper II of this series, we show the application of the present formalism to the study of the mobility versus carrier density in AlGaIn/GaN quantum wells.

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