Intrinsic population inversion in biased multiband superlattices

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The electric field induced carrier redistribution in multiband superlattices is studied within an equation of motion analysis of the density matrix. Semiclassical intrasubband and quantum-mechanical tunneling contributions are identified. It is shown that there is no global population inversion for superlattices with only two minibands. However, we predict that an intrinsic global population inversion may occur at particular electric field strengths in superlattices with at least three minibands. Conditions under which global population inversion is expected to emerge are discussed. It is proposed to exploit the global population inversion that may appear due to resonant tunneling into a wide third miniband to fabricate unipolar midinfrared semiconductor lasers without any injector regions.

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Recently, semiconductor lasers based on an early proposal by Kazarinov and Suris[1,2] to exploit intersubband transitions in quantum wells have been fabricated.[3] In these unipolar midinfrared lasers, called quantum-cascade lasers (QCL's), electrons are injected from contacts to a sequence of active regions alternated with carrier injectors. The wave functions of the excited and ground states of the fundamental optical transition are usually localized in a series of coupled quantum wells that form the active region. The injector minibands remove or inject carriers from the active region via resonant tunneling.[4–8] An alternative concept of generating infrared laser radiation exploits the electronic transitions between minibands in a superlattice (SL). In these structures the applied electric field is compensated by an appropriate variation of the SL period so that flat minibands with well delocalized states are formed. The application of these so called chirped SL's enhances the temperature and power performance of the devices.[9–13] It is a common feature of the above mentioned midinfrared lasers that electrons injected from contacts cascade down alternating injector and active regions to realize local population inversion in the active layers of the laser. In this paper, we propose an alternative concept that allows achievement of an intrinsic *global* population inversion in specifically prepared SL's subject to strong external electric fields. This mechanism is based on resonant tunneling into a wide third miniband.

Resonant tunneling in multiband SL's and its influence on the population of the minibands will be studied within a quantum-kinetic theory. Unlike former approaches,[1,2,14–17] we focus on resonant tunneling and underline the importance of the bandwidth of the uppermost miniband and the scattering induced width of the tunneling resonance to achieve population inversion in a three-band model at the resonance field strength. Our main objective in this paper is the discussion of conditions under which an intrinsic global population inversion is realized in SL's to which a strong electric field is applied.

We start our consideration of the carrier population by treating the standard tight-binding Hamiltonian of a multiband SL in a static electric field E. Nearest neighbor hopping results in the widths Δ_ν (with ν being the miniband index) of isolated field-independent ($E=0$) minibands exhibiting a cosine shaped wave-vector dependence. From the Liouville equation, quantum-kinetic equations are derived for the Wigner transformed elements of the density matrix $f_\nu^{\nu'}(\vec{k})$ ($\vec{k}$ is the wave vector), whose explicit spatial dependence describing field domain formation is not taken into account.[18,19] These equations encompass both scattering-induced electron transitions and quantum-mechanical tunneling. Tunneling is associated with the off-diagonal elements of the density matrix and with the dipole matrix elements $Q_{\nu\nu'}$ calculated from the overlap of SL envelope functions. Besides tunneling transitions, there are scattering-induced horizontal generation and recombination processes characterized by the relaxation times $\tau'_{\nu\nu'}$ and $\tau''_{\nu\nu'}$, respectively. In the description of these transitions, the diagonal elements of the density matrix are involved. In addition, there are scattering-induced vertical transitions, which are associated with the off-diagonal elements of the density matrix and which determine the linewidth of the tunneling resonance. The respective scattering times are denoted by $\tau^{(\nu)}$. In this paper, scattering will be considered in the constant relaxation time approximation.[18,19] Although the heating of the lateral electron motion is neglected in such an approach, the main physics of the problem is preserved. This has been demonstrated by numerous theoretical treatments of QCL's. To stimulate the search for analytic solutions, we transform the kinetic equations into the Wannier-Stark (WS) ladder representation by introducing a Fourier series representation of the density matrix[18] with respect to k_z, which is the component of the wave vector along the SL axis. The electric field is aligned along this direction. Under the influence of high electric fields, the mean Fourier component $f_\nu^{\nu'}(\vec{k}_\perp, l=0)$ dominates over contributions with $l\neq 0$ (l is any integer).

In the case of isolated single minibands, our approach reproduces the extended Esaki-Tsu model studied by Suris and Shchamkhalova.[20] It is known that this model is able to describe the general features observed in optical and transport measurements.

In order to study resonant tunneling, let us first treat a simple two-band model. Under the assumption that at high electric fields the carriers are strongly localized in single wells $[f_\nu^\nu(\vec{k}_\perp, l \neq 0) \ll f_\nu^\nu(\vec{k}_\perp, l=0)]$, we obtain the following analytical result for the occupation probability $f_2 = \Sigma_{\vec{k}_\perp} f_2^2(\vec{k}_\perp, 0)$ of the upper miniband:

$$f_2 = \frac{2\Omega^2 \tau^{(1)} A_{12} + 1/\tau'_{12}}{4\Omega^2 \tau^{(1)} A_{12} + 1/\tau'_{12} + 1/\tau''_{21}}, \tag{1}$$

where $\Omega = eEd/\hbar$ is the Bloch frequency of a SL with the period d and A_{12} is a field-dependent function that describes the tunneling resonances,

$$A_{12} = \left(\frac{Q_{12}}{d}\right)^2 \sum_{l=-\infty}^{\infty} \frac{q_{12}(l)^2}{(l\Omega\tau^{(1)} - \omega_{21}\tau^{(1)})^2 + 1}. \tag{2}$$

The matrix element $q_{12}(l)$ given by

$$q_{12}(l) = J_l\left(\frac{\Delta_1 + \Delta_2}{2\hbar\Omega}\right) \tag{3}$$

exhibits an oscillatory field dependence according to the Bessel function J_l. In the absence of thermal generation $(\tau'_{12} \to \infty)$ and under the condition $f_2 \ll 1$, Eqs. (1)–(3) lead to the result $f_2 \approx 2\Omega^2 \tau^{(1)} \tau''_{21} A_{12}$, which was already derived and discussed previously.[18] Here we are more interested in the case when the occupation of the different minibands f_2 and $f_1 = 1 - f_2$ becomes comparable in magnitude. According to Eq. (2), the tunneling resonance appears when the centers of the minibands are aligned, i.e., when $l\hbar\Omega = \hbar\omega_{21} = \varepsilon_{g1} + (\Delta_1 + \Delta_2)/2$, where ε_{g1} denotes the gap between the minibands. The width of the resonance is scattering mediated only via $\tau^{(1)}$. The absence of an intrinsic tunneling time implies that the tunneling resonance will become arbitrarily sharp when scattering processes are switched off. In contrast, in SL's with narrow minibands $(\Delta_i \to 0)$, when tunneling is increasingly hindered by thick potential barriers, only the $l=0$ component of $q_{12}(l)$ survives, and the tunneling resonance disappears. The most important conclusion from Eq. (1) is that there is no global population inversion in a model with two minibands ($f_2 < 0.5$ because recombination is always faster than generation $\tau''_1 < \tau'_1$). This result, which is in conflict with the assertion made by Kazarinov and Suris,[2] is confirmed by an exact numerical solution of the kinetic equations. In this numerical study field-induced resonance tunneling is treated exactly. An example of the numerically calculated field-dependent miniband occupations is shown in Fig. 1. The dashed line has been calculated from Eqs. (1)–(3). Sharp tunneling resonances occur at ω_{21} and $\omega_{21}/2$. For the set of parameters used, the occupation of the upper miniband reaches nearly its maximal value of 0.5 at the resonance $\Omega = \omega_{21}$. The weaker tunneling resonance at $\Omega = \omega_{21}/2$ is due to tunneling between next-nearest WS levels. The exact numerical solution of the kinetic equation,

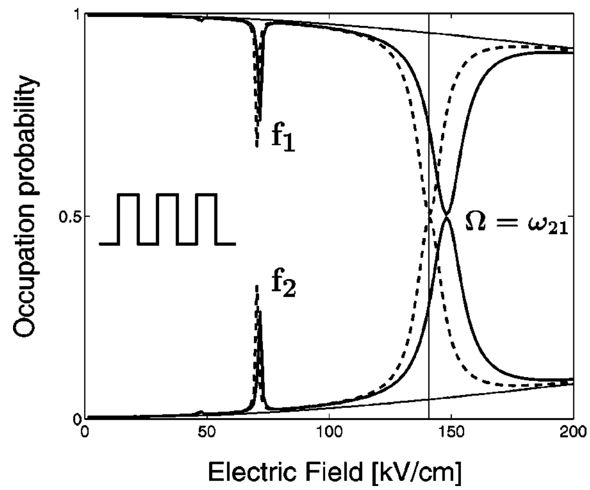

FIG. 1. Occupation probability f_1 (f_2) of the lower (upper) miniband as a function of the electric field strength for $\Delta_1 = 2$ meV, $\Delta_2 = 80$ meV, and $\varepsilon_g = 100$ meV. For the tunneling times $\tau^{(1)}$ and τ''_{21} we used 1 ps. The scattering time τ'_{12} for carrier generation was determined via the principle of detailed balance at $T = 300$ K. The dashed line has been calculated from Eqs. (1)–(3). The thin solid line is the result for narrow minibands $(\Delta_1, \Delta_2 \to 0)$ and the thick solid line exhibits the exact result. The intrasubband scattering times τ_1 and τ_2 are needed for the exact numerical calculation. As an example, we used $\tau_1 = 0.2$ ps and $\tau_2 = 0.7$ ps. An estimate for the dipole matrix element was obtained from a quantum well with infinitely high barriers $(|Q_{12}|/d = 1/2\pi)$. The SL period is $d = 10$ nm. The inset illustrates the periodic potential.

shown by the thick solid line, exhibits quite similar behavior. The main discrepancy between the analytical result (dashed line) and the exact numerical data (thick solid line) consists in a renormalization of the tunneling resonance position at $\Omega = \omega_{21}$ due to transitions between different WS levels described by $f_\nu^{\nu'}(\vec{k}_\perp, l \neq 0)$. In the limit of narrow minibands $(\Delta_1, \Delta_2 \to 0)$, the tunneling resonances completely disappear as shown by the thin solid line.

In contrast to the two-band model, a SL with at least three minibands may exhibit an intrinsic global population inversion. As an example, let us consider a SL made of a 2 nm thick, 250 meV high barrier surrounded by 5 nm thick barriers the height of which amounts to 50 meV. These symmetric barriers are separated by 8 nm thick wells. The energy dispersion relation of this SL model calculated at vanishing electric fields $(E=0)$ is shown in Fig. 2. Three minibands are formed, the dispersion relations of which are approximated in our calculation by cosine functions. The derivation of kinetic equations for the SL with three minibands is straightforward and follows the same line of argument as in Ref. 18. For the three-band model, the set of coupled kinetic equations enlarges considerably, and it is difficult to derive analytical solutions that cover a large interval of the electric field strength. Nevertheless, we can simplify the treatment of resonant tunneling by taking into account the fact that in the most interesting high field region and under the condition $\varepsilon_{gi} \gtrsim \Delta_i$ the transitions between different Stark ladder states play only a minor role $[f_\nu^\nu(l \neq 0) \ll f_\nu^\nu(l=0)$ with $f_\nu^\nu(l) = \Sigma_{\vec{k}_\perp} f_\nu^\nu(\vec{k}_\perp, l)]$.

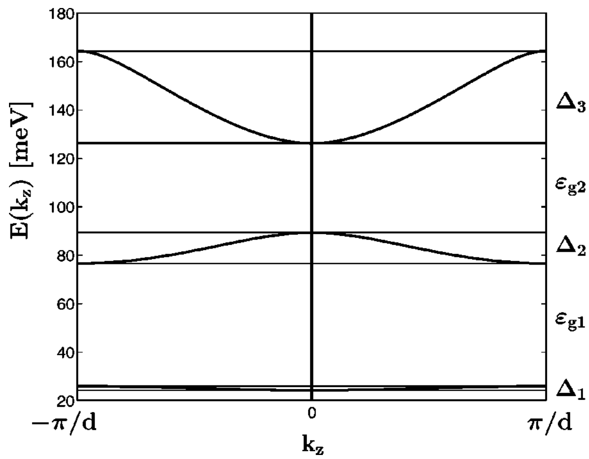

FIG. 2. Energy dispersion relation for a SL with an 8 nm thick well and a barrier that consists of three blocks: (1) 5 nm, 50 meV, (2) 2 nm, 250 meV, and (3) 5 nm, 50 meV. The energy gaps and miniband widths are indicated on the right hand side.

Figure 3 shows an example of the field-dependent carrier redistribution for a SL with three minibands as numerically calculated from the coupled set of kinetic equations. The unbiased SL is characterized by the energy dispersion relation shown in Fig. 2. The redistribution of carriers exhibits a dramatic field dependence at 58 kV/cm, where the lowest and uppermost WS levels of adjacent wells are aligned to each other by the electric field. Resonant tunneling leads to a

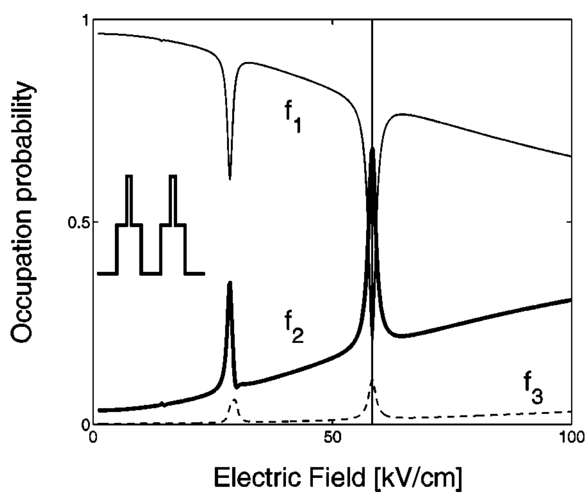

FIG. 3. Field dependence of the occupation probabilities $f_i(f_1+f_2+f_3=1)$ for a superlattice with three minibands. The SL at zero bias is characterized by the energy dispersion relation shown in Fig. 2, from which the energy gaps and miniband widths are obtained ($\varepsilon_{g1}=50$ meV, $\varepsilon_{g2}=35$ meV, $\Delta_1=2$ meV, $\Delta_2=12$ meV, and $\Delta_3=37$ meV). It is assumed that the scattering times for vertical transitions, which determine the width of the tunneling resonance, are all equal ($\tau^{(1)}=\tau^{(2)}=\tau^{(3)}=1$ ps). Furthermore, we used the following relaxation times for carrier recombination: $\tau''_{21}=\tau''_{31}=1$ ps and $\tau''_{32}=0.1$ ps. The lattice temperature is 300 K. The thin vertical line indicates the position of the tunneling resonance ($\Omega=\omega_{31}$) at which population inversion occurs between the lowest miniband and the first band of excited states. The inset illustrates the periodic potential.

population inversion between the occupations $f_1=f_1^1(l=0)$ and $f_2=f_2^2(l=0)$. The resonance condition $\hbar\Omega=\hbar\omega_{31}=\varepsilon_{g1}+\varepsilon_{g2}+\Delta_2+(\Delta_1+\Delta_3)/2$ implies that resonant tunneling occurs when the centers of the first and third minibands are aligned. Another interesting observation is that the width of the tunneling resonance is not directly related to the widths of the minibands involved. In fact, there is no intrinsic tunneling time. The width of the tunneling resonance is induced by scattering. A second tunneling resonance occurs at 29 kV/cm, when the first and third WS levels of next-nearest neighbors are aligned by the electric field ($\Omega=\omega_{31}/2$). This pronounced resonance does not give rise to any population inversion for realistic parameter sets.

To better understand the conditions that lead to the population inversion, let us derive analytical results valid in the vicinity of the tunneling resonance. For electric fields satisfying the resonance condition $\Omega\approx\omega_{31}$ and neglecting the small contributions due to carrier generation, we obtain from the kinetic equations the solution $f_2=f_3\tau''_{21}/\tau''_{32}$, $f_1+f_2+f_3=1$, and

$$f_2=\frac{\tau''_{21}}{\tau''_{32}}\frac{2\Omega^2\tau^{(2)}A_{13}}{2\Omega^2\tau^{(2)}(2+\tau''_{21}/\tau''_{32})A_{13}+1/\tau''_{31}+1/\tau''_{32}}, \tag{4}$$

where A_{13} is given by Eq. (2) with Q_{12}, q_{12}, ω_{21}, and $\tau^{(1)}$ being replaced by Q_{13}, q_{13}, ω_{31}, and $\tau^{(2)}$, respectively. The field-dependent function q_{13} is expressed by the Bessel function

$$q_{13}(l)=J_l\left(\frac{\Delta_3-\Delta_1}{2\hbar\Omega}\right). \tag{5}$$

From the analytical solution of the kinetic equations, we obtain that an intrinsic global population inversion ($f_2>f_1$) occurs when the following inequality is satisfied:

$$\frac{1}{\tau''_{31}}+\frac{1}{\tau''_{32}}<2\left(\frac{Q_{13}}{d}\right)^2\omega_{31}^2\tau^{(2)}\left(\frac{\tau''_{21}}{\tau''_{32}}-1\right)J_1\left(\frac{\Delta_3-\Delta_1}{2\hbar\omega_{31}}\right)^2. \tag{6}$$

Physically it is evident that the occurrence of the inversion requires $\tau''_{21}>\tau''_{32}$, which means that carriers quickly vacate the uppermost miniband via an effective scattering channel (e.g., via longitudinal optical phonon emission), whereas the subsequent recombination to the ground state proceeds more slowly. Similarly, the occupation of the excited states could be inverted at the resonance field strength when the second subband is emptied faster than the third one ($\tau''_{32}>\tau''_{21}$). This is the most important criterion for the appearance of population inversion. However, as seen from Eq. (6), this condition is not sufficient. In narrow band SL's ($|\Delta_3-\Delta_1|\to 0$), an intrinsic global population inversion cannot occur because the value of the Bessel function goes to zero. This simply means that tunneling becomes ineffective in the sequential tunneling limit ($|\Delta_3-\Delta_1|/2\hbar\omega_{31}\ll 1$). According to Eq. (6), a wide uppermost miniband favors population inversion due to resonant tunneling. To our knowledge, this is an essential criterion for the design of injectorless QCL's based on an intrinsic global population inversion due to resonant tunneling in SL's not proposed before. One possibility for realizing SL's of this kind is to grow barriers with a thin central layer that allows the formation of a wide third miniband. For extremely large miniband widths, when ε_{g1} and ε_{g2} are much smaller than Δ_3, our approach becomes inapplicable. However, this limit is irrelevant for QCL applications. As the finite width of the minibands is decisive, midinfrared lasers based on the described resonant tunneling mechanism cannot be realized with multiple quantum wells, which do not exhibit any minibands.

There is another mechanism that essentially affects the formation of population inversion. This is the scattering-induced broadening of the tunneling resonance described by $\tau^{(2)}$ in Eq. (4). In the limit $\tau^{(2)}\rightarrow 0$, the tunneling resonance is smeared out, and the population inversion disappears. In contrast, when the scattering time $\tau^{(2)}$ becomes too large to fulfill the inequality (6), an extremely sharp tunneling resonance arises so that any misalignment of the WS states by the electric field destroys the population inversion. Therefore, an intermediate value of $\tau^{(2)}$ is applicable.

In summary, we have considered the carrier redistribution due to resonant tunneling in biased multiband SL's on the basis of a quantum-kinetic approach. We arrived at the conclusion that an intrinsic global population inversion can occur only in SL's with at least three minibands due to resonant scattering under the influence of strong applied electric fields. Crucial for the appearance of the inversion is the requirement that the relaxation from the uppermost miniband into the intermediate subband proceeds faster than the relaxation from the latter into the ground state. But this criterion is not sufficient. An intrinsic global population inversion due to resonance tunneling in SL's can emerge only when the uppermost miniband is sufficiently wide. We think that this is an essential criterion for the fabrication of midinfrared lasers that exhibit an intrinsic global population inversion based on resonant tunneling in SL's.

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