Sequential resonant tunneling in quantum cascade lasers

Romain Terazzi, Tobias Gresch, Andreas Wittmann, and Jérôme Faist
Quantum Optoelectronics Group, Institute for Quantum Electronics, ETH, 8086 Zürich, Switzerland

A model of sequential resonant tunneling transport between two-dimensional subbands that takes into account explicitly elastic scattering is investigated. It is compared to transport measurements performed on quantum cascade lasers where resonant tunneling processes are known to be dominating. Excellent agreement is found between experiment and theory over a large range of current, temperature and device structures.

Resonant tunneling in semiconductor heterostructures has motivated a large number of experimental and theoretical studies. One of the most studied case is the resonant tunneling diode, where a quantum well is formed by a double-barrier region. Under a variable applied electric field, the transparency of the system is probed by coherent tunneling of electrons at the Fermi energy of the contact region. The voltage-current curve exhibits a clear maximum when the emitter electrode aligns with a resonance of the well. This perfect case might be realised when the exit barrier is made so thin that the escape tunneling rate is much faster than other dephasing mechanisms. Because of strong in-plane scattering this condition is difficult to achieve. Usually current proceed by sequential tunneling as it is the case in quantum cascade lasers.

In the pioneer work of Kazarinov, the current is expressed in a density matrix model where the resonance curve is found lorentzian with an homogeneous broadening given by the average value of elastic scattering matrix elements. As a consequence of the averaging the electrons tunnel between subbands conserving their in-plane wavevectors.

More recently a refined model that include previously averaged-out second-order mechanisms was developed. Second order scattering is known to yield gain without a net population inversion through scattering assisted optical transitions, but it also affects more generally resonant tunneling, by allowing transitions between subband states of different wavevectors. It is found that resonant tunneling occurs with conservation of the energy rather than the wavevector, contrarily to the first order case.

In this letter we demonstrate the important role played by second order mechanisms in sequential resonant tunneling and therefore in the carrier transport of semiconductor heterostructures.

When second order terms are considered in the calculation, the current density between a pair of subbands coupled through a barrier is expressed as:

\[
\frac{J}{d} = e\Omega^2 \sum_k \frac{\gamma_k^i \left( f_{k^+_2} - f_{k^+_1} \right) + \gamma_k^e \left( f_{k^-_2} - f_{k^-_1} \right)}{\Delta^2 + \left( \gamma_k^i + \gamma_k^e \right)^2}
\]

(1)

with \(q_k = \hbar \sqrt{2m^* (\epsilon_k \pm \Delta)}\), where \(f_k^n\) is the carrier distribution in subband \(i\) at wavevector \(k\), \(\Delta\) is the detuning between the subband edges \(\Delta = \epsilon_2 - \epsilon_1\), \(\hbar \Omega\) is the coupling energy through the barrier, \(d\) is the difference between the two centroids of the wavefunctions \(d = z_2 - z_1\), \(e\) is the elementary charge and \(\gamma_k^i\) is the broadening of state \(i\) at wavevector \(k\).

When a low density of electrons is distributed thermally in each subband, with the same electronic temperature \(T\) and that a same and uniform scattering potential is considered (\(\gamma_k^i = \gamma_k^e = \gamma\)), the current density can be integrated and simply rewritten as:

\[
\frac{J}{d} = \frac{e\Omega^2 2\gamma}{\Delta^2 + (2\gamma)^2} \left\{ \theta(\Delta) \left( n_2 - e^{-\beta\hbar|\Delta|} n_1 \right) + \theta(-\Delta) \left( e^{-\beta\hbar|\Delta|} n_2 - n_1 \right) \right\}
\]

(2)

where \(\theta(x)\) is the Heaviside function, with \(\theta(x^-) = 0, \theta(x^+) = 1\) and \(\theta(0) = \frac{1}{2}, \beta = 1/kT\) with \(k\) the Boltzmann constant and \(n_i\) is the net population of subband \(i\).

The current density is no more driven by the population difference \(n_2 - n_1\) but by an effective population term. We want to examine two extreme case: equally populated subbands \(n_2 = n_1 = n\) and one empty subband \(n_1 = 0\). The first case is shown in Fig. (a). The current density is dispersive shaped around the resonance. A negative current peak occurs when the detuning is negative, this is when the edge of subband 1 is above the edge of subband 2. When the subbands are aligned the current is zero and the first order approximation is recovered. The current then turns to be positive, after the edge of subband 2 has overcome the edge of subband 1, this is when the detuning is positive. The
A dispersive shape is the consequence of electron tunneling at a constant energy rather than at a constant wavevector. As shown in Fig. 1(a) the first order model yield a zero current for any detuning. This case illustrate a superlattice: the current is zero until second-order scattering terms have been taken into account.

The case where one subband is empty is shown in Fig. 1(b). For negative detunings the current between the subbands is exponentially reduced as only the electrons with a sufficient kinetic energy are able to tunnel to subband 1. Contrarily, for positive detunings, the first and second order curves overlap perfectly as all electrons are above the edge of subband 1.

Generally the first order model is recovered as the thermal energy largely overcomes the detuning energy $kT \gg \hbar|\Delta|$, as it is the case in Eq. 2. In Eq. 2 the exponential cut-off tends to 1 as the temperature tends to infinity, spreading electrons in an uniform distribution.

As second order mechanisms strongly affect the resonant current between a pair of subbands, we aim to show its impact on more complex semiconductor heterostructures like quantum cascade lasers. We therefore have implemented second-order effects in the computation of the voltage-current characteristic.

The computational model is based on the density matrix where dissipation is included as rate equations for the populations and as dephasing times for the polarisations. The precise implementation will be detailed elsewhere. A typical quantum cascade laser is a repetition of a fundamental period as shown in Fig. 2. These periods are coupled through an injection barrier. Electrons are injected by sequential resonant tunneling from a period to the next one. The period itself can be separated in an active region where the laser transition occurs and an injector region where carriers are relaxed before they are injected into the next period. For many structures, and the ones presented here, the active region is coupled to the injector region through an extraction barrier as shown in Fig. 2. We therefore have implemented tight-binding and sequential resonant tunneling at the injection and at the extraction barrier. In the active region and the injection region, the carriers are relaxed through intersubband scattering. The mechanisms we have considered include LO-Phonons, interface roughness and ionized impurities.
(dopants) scattering. Non-parabolicity effects and self-consistency of the potential are accounted by the model. A uniform electronic temperature is computed for all subbands, based on the electron energy balance. The numerical simulations output the populations of the subbands and the current density flowing through the heterostructure. We are therefore able to predict the voltage-current characteristic of a particular quantum cascade structure. In order to test the impact of second order transport, we have implemented both first and second order sequential resonant tunneling models.

We present two quantum cascade structures in different coupling regimes. The first show in Fig. 2(a) has a strong coupling between the active and the injector regions as the extraction barrier is made sufficiently thin (22 Å). Contrarily...

**FIG. 2:**
Each structure is shown at injection resonance field. The layer sequence starts from the injection barrier and the thicknesses are in nm; roman, resp. bold, numbers indicate In$_{0.53}$Ga$_{0.47}$As, resp. Al$_{0.48}$In$_{0.52}$As alloy, acting as well, resp. barrier material. (a) Layers: 4.3/1.7/0.9/5.4/1.1/5.3/1.2/4.7/2.2/4.3/1.5/3.8/1.6/3.4/1.8/3.0/2.1/2.8/2.5/2.7/3.2/2.7/3.6/2.5. Underlined layers are 1.5 × 10$^{17}$ cm$^{-3}$ Si doped. Nominal sheet carrier density is 1.2 × 10$^{11}$ cm$^{-2}$. Period length is 68.3 nm, repeated 35 times. The optical transition occurs at ≈154 meV. (b) Layers: 4.8/3.6/0.2/3.6/3.5/5.1/1.1/5.0/1.2/4.5/1.3/3.5/1.5/3.4/1.6/3.3/1.8/3.2/2.1/3.0/2.5/3.0/2.9/2.9. Underlined layers are 3 × 10$^{17}$ cm$^{-3}$ Si doped. Nominal sheet carrier density is 3.03 × 10$^{11}$ cm$^{-2}$. Period length is 68.6 nm, repeated 35 times. The optical transition occurs at ≈167 meV.
in Fig. 2(b) the second structure is a single quantum well as its active region is formed by one well only, weakly coupled to the injector region by a thick extraction barrier (30 Å).

FIG. 3:

The current curves are shown both in log scale (left axis) for inspection of low currents and in linear scale (right axis) for inspection of the dynamic range. (a) Experimental data (full line), simulation with second order resonant tunneling (dotted line), simulation with first order model (dashed line). (b) Single quantum well current-voltage curves for three temperatures: 80 K, 180 K and 300 K. Measurements displayed in full line. Simulations in broken line.

The current-voltage curves for both structures are shown in Fig. 3. The measurements are taken in continuous mode for low currents and in pulsed mode when current flow causes a heating of the sample. The cryostat temperature for the first sample is 300 K, while it is 80 K, 180 K and 300 K for the second.

In Fig. 3(a) the second order voltage-current curve fits the experimental data much better than the first order approximation from the very low currents to the maximal current.

If we focus on the low field values of the voltage-current curve, the second order model clearly better predicts the experimental behaviour than the first order model does. In particular it yields a zero net current at zero field which is an important validation of the computational model.

The result for the single quantum well structure are shown in Fig. 3(b). We have shown simulated curves with second order model only, because the first order model failed to converge at low fields values and is largely off from the measurements. Apart from a constant serial resistance (0.5 Ω) than higher systematically the experimental bias, the model was able to reproduce nicely the experiment, in particular for high temperature where the transport in the structure is clearly dominated by optical phonons. The model predicts the low temperature curve with less accuracy.
because the transport at such a temperature also require the computation of scattering rates due to acoustical phonons and electron-electron interactions, which are not computed in the present model.

Agreement between computed and experimental current-voltage characteristics has already been reported for other model approaches such as based on Monte Carlo or non-equilibrium Green’s functions, the comparison was done however on a much more limited range of currents, temperature and structure design.

Formally, the current driven by tunneling between two subbands through a barrier or by optical absorption are physically equivalent because both processes conserve the in-plane wavevector. As a result, the striking agreement between the predictions of the second-order model and the experiment can be interpreted as a strong experimental evidence for the validity of the Bloch gain model.

This work was supported by the Swiss National Science Foundation, the National Center of Competence in Research, Quantum Photonics and the Swiss Commission for Technology and Innovation.

---

1. P. Guérét, C. Rossel, and H. Meier, J. Appl. Phys. 67, 900 (1990).
2. T. Ihn, H. Carmona, P. Main, L. Eaves, and M. Henini, Phys. Rev. B 54, 2315 (1996).
3. J. Eisenstein, T. Gramila, L. Pfeiffer, and K. West, Physical Review B 44 (1991).
4. H. Willenberg, G. Döhler, and J. Faist, Phys. Rev. B 67, 085315 (2003).
5. R. Terazzi, T. Gresch, M. Giovannini, N. Hoyler, N. Sekine, and J. Faist, Nature Phys. 03, 329 (2007).
6. A. Wacker, Advances in Solid State Physics pp. 199-210 (2001), cond-mat/0105312.
7. R. Kazarinov and R. Suris, Sov. Phys. Semicond. 6, 120 (1972).
8. J. Faist, F. Capasso, D. Sivco, C. Sirtori, A. Hutchinson, and A. Cho, Science 264, 553 (1994).
9. R. Terazzi (2008), unpublished.
10. T. Unuma, M. Yoshita, T. Noda, H. Sakaki, and H. Akiyama, J. Appl. Phys. 93, 1586 (2003).
11. S. Tsujino, A. Borak, E. Müller, M. Scheinert, C. Falub, H. Sigg, D. Grützmacher, M. Giovannini, and J. Faist, Appl. Phys. Lett. 86, 062113 (2005).
12. P. Harrison, D. Indjin, and R. Kelsall, J. Appl. Phys. 92, 6921 (2002).
13. H. Callebaut and Q. Hu, Journal of Applied Physics 98, 104505 (2005).
14. A. Wacker, Physical Review B 66, 085326 (2002).