Quantum cascade lasers (QCLs) [1] are semiconduc-
tor unipolar devices emitting coherent infrared radiation. Their active regions consist of stacked planar quantum wells (QWs) forming a superlattice along the growth di-
rection. At first sight, a large part of the physical prop-
ties of QCLs can be qualitatively understood in a one-
dimensional picture, in particular for quantum confine-
ment, tunneling processes and radiative transitions. Nev-
evertheless, the free in-plane motion of the carriers provides a continuous energy reservoir (i.e. subbands) which plays a major role in the energy and phase relaxation processes. For QCLs operating in the terahertz (THz) range [2–3], due to the relatively small energy separation between the subbands associated with the lasing levels, the non-
radiative scattering processes are very efficient and are responsible for intrinsic limitations in terms of quantum efficiency and maximum operation temperature.

Reducing the dimensionality of electronic systems is generally a way to increase the carrier lifetimes [4–7]. A strong magnetic field applied along the growth axis of a QCL quantizes the lateral motion in terms of Landau levels. Their energy tuning with magnetic field has been shown to be responsible for modulation of the level lifetimes [8–9], allowing to demonstrate lasing up to higher temperature (225 K in ref. [10]) than in usual THz QCLs (199 K in ref. [11]). However, Landau levels remain highly degenerate so that their ideal discrete density of states is strongly broadened by disorder effects [12]. On the other hand, QCLs based on 0D nanostructures such as self-assembled or lithographically defined quantum dots (QDs) have been proposed [13–16] in order to achieve low threshold current and high operation temperature. However, a clear comparison of the device performances with respect to conventional THz QCLs is still lacking, and the intermediate regime between coupled 0D QDs and coupled 2D QWs remains to be investi-
gated.

In this letter we propose a novel type of QCLs based on nanowire (NW) superlattice heterostructures. Within the formalism of non-equilibrium Green functions (NEGF), we present a theory of dissipative quantum dy-
namics in wire axial superlattices, which provides a uni-
fied model of electron transport and THz gain in super-
lattices with and without lateral dimensional quantum effects. We investigate the modifications in the scattering mechanisms and in the nature of charge transport associated with the transition from the 2D to the 0D limits for the lateral motion. Our calculations demonstrate that below a critical thickness NW THz QCLs have the ability to achieve higher temperature operation and lower current threshold than conventional THz QCLs.

The active region of the proposed QCL consists of an array of parallel NWs, each of them containing a superlattice heterostructure along the growth axis. The ex-
perimental realization could be done either by etching of a standard QCL heterostructure or by a bottom-up ap-
proach. The electronic structure is modeled within the ef-
ective mass approximation. The NW surface is assumed to be perfectly passivated so that no charge depletion or accumulation effects occur. We consider an electron wave function basis set of the form $\psi_{\alpha n} = \psi_n(z) \phi_\alpha(\rho, \theta)$, where $\phi_\alpha$ are the solutions of the Schrödinger equation on a homogeneous disc (the assumed NW cross-section) with eigenvalues $E_n$ and the $\psi_n$ form a periodic basis set of the low energy states along the $z$ superlattice axis [17].

The electron dynamics is calculated within the NEGF formalism in which the perturbative scattering processes are treated within the self-consistent Born approxima-
tion (SCBA). Self-consistent (SC) NEGF implementa-
tion of dissipative quantum transport in semiconduct-
heterostructures [18–21] allows a coherent and non-
Markovian treatment of the charge dynamics, where the scattering self-energies can be conveniently treated on a microscopic basis. In the present work, a SC-NEGF for-
malism is further required since dimensionality transition is intrinsically a self-consistent problem between scattering processes and line broadening effects. The electron lesser Green function (GF) reads $G_{\alpha, \beta, \sigma, \tau}(t_1, t_2) = \langle a_{\beta, \tau}^\sigma(t_2) a_{\alpha, \sigma}(t_1) \rangle$, where $a^\dagger_\alpha$ ($a_\alpha$) are the electron creation (annihilation) operators, $\alpha$ and $\beta$ referring to the $\psi(z)$
modes and $n$ to the $\phi_n(r, \theta)$ disk eigenstates. Thus coherences (i.e. $\alpha \neq \beta$) are considered in the growth direction while only populations are considered for the lateral modes. Field-periodic boundary conditions [19] are applied.

We take into account the scattering mechanisms that are known to be important in QW QCLs heterostructures: longitudinal optical (LO) and acoustical phonon emission/absorption, interface roughness, charged impurities and alloy disorder. In addition, scattering mechanisms specific to NW and/or quasi 0D systems are also considered. The NW surface roughness is taken into account as an additional elastic scattering mechanism. NW phonon confinement effects are considered and we calculate the coupling of electrons to longitudinal optical (LO) and surface optical (SO) phonons [22], as well as confined acoustic phonons.

In quasi 0D systems, early studies have predicted a phonon bottleneck as soon as discrete electronic transitions are detuned from the optical or acoustical phonon frequencies [11] [23]. More recent studies have demonstrated that (i) direct LO-phonon emission/absorption processes are totally suppressed even in case of electron–LO-phonon resonances due to the strong coupling regime between electrons and LO-phonons [24], and that (ii) the dominant energy relaxation of terahertz excitations is the polaron anharmonicity, i.e. an indirect scattering process involving electron–LO-phonon polar interaction as well as anharmonic couplings of LO-phonons with other phonon modes [5, 7, 25]. In the present case, we have checked that the SCBA very well reproduces the polaron anharmonicity, i.e. an indirect scattering process involving electron–LO-phonon polar interaction as well as anharmonic couplings of LO-phonons with other phonon modes [5, 7, 25]. In the present work, we have generated random correlated potentials $\bar{V}_{nn}(z)$ for an incoherent treatment of the disorder effects. Here, as the NW gets thinner, the elastic scattering becomes mainly coherent, as the disorder potential fluctuations become larger than the phonon-limited broadening. In the present work, a coherent treatment of the disorder potential $V$ within each lateral channel $V_{nn}(z) = \langle \phi_n | V | \phi_n \rangle$ is achieved. For this purpose, we generate random correlated potentials $V_{nn}(z)$ from the principal component analysis of the covariance matrix $(V_{nn}(z)V_{nm}(z'))$.

The elastic scattering mechanisms induced by disorder effects (here interface roughness, surface roughness, alloy disorder and charged impurities) are usually treated within the SCBA in planar QW heterostructures [18] [19] [21]. However, the SCBA only accounts for an incoherent treatment of the disorder effects. Here, as the NW gets thinner, the elastic scattering becomes mainly coherent, as the disorder potential fluctuations become larger than the phonon-limited broadening. In the present work, a coherent treatment of the disorder potential $V$ within each lateral channel $V_{nn}(z) = \langle \phi_n | V | \phi_n \rangle$ is achieved. For this purpose, we generate random correlated potentials $V_{nn}(z)$ from the principal component analysis of the covariance matrix $(V_{nn}(z)V_{nm}(z'))$.

On the other hand, the elastic scattering between different lateral eigenmodes remains treated within the SCBA and corresponding lesser/retarded self-energies read $\Sigma_{<,R}(E) = \sum _{m \neq n} \langle \phi_m | V_{nm}(z) | \phi_n \rangle G_{nm}^{<,R}(E)$. The transport and optical properties are calculated for each random potential realization and finally averaged.

We consider here the In$_{0.53}$Ga$_{0.47}$As/GaAs$_{51}$Sb$_{49}$ material system lattice matched to InP, in which a conventional THz QCL operating up to 142 K has recently been demonstrated [26]. This system could be used to realize NW QCLs in a top-down approach, and bottom-up approaches may also be possible with similar material systems [27] [28]. We consider below 3-well resonant phonon designs (A and B), similar to the one holding operation temperature records in conventional THz QCLs [11]. The layer sequence in nanometers of the design A is 14/1.5/11.2/3.5/22/3.5 with barriers indicated in bold fonts and the doped layer underlined. The equivalent areal doping density per period is set to $3 \times 10^{10}$ cm$^{-2}$. The interface and surface roughnesses are both assumed to have a rms fluctuating amplitude of 3 Å with correlation lengths of 8 nm. The filling factor of the NW array is assumed to be unity for simplicity in the treatment of Coulombic interactions and for clear comparison with the conventional QCL geometry.

Fig. [4] shows the calculated transport properties of the NW QCLs. The current–voltage characteristics calculated for various NW diameters at room temperature are shown on Fig. [1(a)]. Fig. [1(b)] shows the current density as a function of the NW diameter for a fixed applied bias of 65 mV per period for various temperatures. For sufficiently thick wires the calculated current densities saturate on Fig. [1(b)] and all the IV curves for diameters larger than $150 \text{ nm}$ (not shown on Fig. [1(a)]) overlap. This corresponds to the 2D regime of the lateral motion, i.e. when the lateral quantization effects are negligible. When the NW diameter is reduced below a temperature-dependent critical diameter, variations of the current density are observed on Fig. [1(b)] corresponding to the appearance of lateral dimensional effects. In this quantum wire regime, the I–V characteristic possesses more distinct peaks as the reduction of the scattering processes allows adiabatic
transport over larger distances. In fact, in the 2D regime the lateral motion provides an energy reservoir towards which the excess axial energy is easily transferred via the disorder potentials. As the lateral motion gets quantized, this elastic energy exchange tends to be suppressed. As the remaining scattering processes are mainly due to optical phonons, a strong current peak remains for potential drop per period matching the optical phonon energy (34 meV), whereas the current is strongly reduced for other bias voltage. For thin diameters, as this parasitic current peak at 34 mV becomes larger than the current at the laser operating bias (around 65 meV), electrical instability can occur in the design A. In order to restore electrical stability, designs B differ from the design A mainly by twice thicker injector and extractor tunneling barriers (7 nm instead of 3.5 nm) are investigated. Owing to the sharper tunneling resonances and the effective mass temperature dependence, two slightly different designs B and the design B are studied at respectively 300 K and 100 K. As shown on Fig. 1(a) at 300 K, the weaker tunneling couplings in designs B allow a reduction of the current leakage peak at the optical phonon energy. A further insight into the nature of transport is provided by the analysis of the spectral function (not shown here). For the thick injector and collector barriers in the design A, anticrossings in the spectral function at the tunneling resonances are observed only for NW diameters smaller than ∼35 nm (∼60 nm) at 300 K (100K respectively), indicating than the nature of these resonant tunneling processes evolves from an incoherent to a coherent regime as the NW thickness is reduced.

We calculate the THz gain in linear response with a self-consistent treatment of the induced self-energies (i.e. including vertex corrections) [29], which has been shown to be necessary to correctly treat the correlation in the scattering potentials [30]. The calculated intensity gain spectra at the optimal operating bias are shown on fig. 2 at 300 K, and the peak values of the gain are plotted as a function of the NW diameter at 100 K and 300 K. The gain of the design A in the QW limit reaches 6 cm$^{-1}$ at room temperature, which is below the typical reported cavity losses [31]. The gain strongly in-

FIG. 1: (Color online). Transport properties of the NW QCLs. (a) Current density as a function of the voltage drop per period for various NW diameters at lattice temperature of 300 K, for the design A (solid and dotted lines for respectively stable and unstable operating regions) and for the designs B (dashed-dotted lines). The designed operating bias (65 mV) is indicated by a vertical dotted line. Layer sequences of designs A and B are explicit in the text. (b) Current density as a function of the NW diameter for fixed operating bias voltage at lattice temperatures of 100 K (red lines) and 300 K (black lines) for the design A (solid lines) and the designs B (dashed-dotted lines). The top axis indicates the energy separation between the NW lateral ground state $\phi_0$ and the first excited state $\phi_1$.

FIG. 2: (Color online). Intensity gain spectra at 300 K calculated for various NW diameter for the design A (solid lines) and the design B (dashed-dotted lines).
creases as the NW diameter decreases into the quantum wire regime. Assuming cavity losses equivalent to an absorption of 15 cm$^{-1}$, our calculations predict THz lasing at 300 K for NW diameters smaller than 70 nm. As the NW diameter is further reduced below 38 nm at 300 K (62 nm at 100 K), the design A becomes electrically unstable (dotted lines on Fig. 3). The design B is stable down to thinner NW diameters and its gain for NW diameter between 30 and 36 nm reaches values around 60 cm$^{-1}$ at room temperature, which is equivalent to the calculated value at 100 K in the 2D limit. Below 20 nm diameters, as the lateral extent of the electron wavefunctions becomes comparable with the correlation length of the interface and surface roughnesses, the gain strongly decreases due to the large energy fluctuations and the consequent misalignment of the QCL levels. Interestingly the calculated gain for the designs $B_{300}$ and $B_{100}$ is positive only below a critical diameter (38 nm at 300 K and 100 nm at 100 K), and is negative beyond up to the 2D limit. Indeed, coherent propagation through their large injector and collector tunneling barriers occurs only in the quantum wire regime, whereas in the 2D limit the tunneling is mainly incoherent and not efficient enough to allow population inversion. A further advantage of the designs $B_{300}$ and $B_{100}$ in the quantum wire regime resides in their much smaller current densities threshold (more than one order of magnitude smaller) than the design A operating in the 2D limit.

In summary, we have developed a microscopic dissipative quantum transport theory of electrons in NW superlattices. We have investigated the effects of lateral dimensionality on the physics of electron dynamics and on the THz QCL device performances. We have shown that NW confinement in the active region of THz QCLs is a promising way to achieve room temperature operation. In addition, the increase of the coherent propagation lengths in the quantum wire regime opens the route to designs with larger tunneling barriers and much lower current threshold.

This work has been supported by the Alexander von Humboldt fundation and the Austrian Science Fund FWF (SFB IR-ON). S. Birner, M. Braunstetter, C. Deutsch, P. Greek, G. Kohlbmüller, M. Krall, T. Kubis, S. Rotter, K. Unterrainer and P. Vogl are gratefully acknowledged for fruitful discussions.

FIG. 3: (Color online). Maximum intensity gain as a function of the NW diameter at 300K (black lines) and 100K (red lines) for the design A (solid and dotted lines for respectively electrical stable and unstable gain regions) and for the designs B (dashed-dotted lines, only for NW diameters satisfying electrically stability).
[19] S. C. Lee and A. Wacker, Phys. Rev. B 66, 245314 (2002).
[20] N. Vukmirovic, Z. Ikon, D. Indjin, and P. Harrison, Phys. Rev. B 76, 245313 (2007).
[21] T. Kubis, C. Yeh, P. Vogl, A. Benz, G. Fasching, and C. Deutsch, Phys. Rev. B 79, 195323 (2009).
[22] H. Xie, C. Chen, and B. Ma, Phys. Rev. B 61, 4827 (2000).
[23] H. Benisty, C. M. Sotomayor-Torr`es, and C. Weisbuch, Phys. Rev. B 44, 10945 (1991).
[24] S. Hameau, Y. Guldner, O. Verzelen, R. Ferreira, G. Bastard, J. Zeman, A. Lemaitre, and J. M. Gérard, Phys. Rev. Lett. 83, 4152 (1999).
[25] T. Grange, R. Ferreira, and G. Bastard, Phys. Rev. B 76, R241304 (2007).
[26] C. Deutsch, M. Krall, M. Brandstetter, H. Detz, A. M. Andrews, P. Klang, W. Schrenk, G. Strasser, and K. Unterrainer, Appl. Phys. Lett. 101 (2012).
[27] L. Samuelson, C. Thelander, M. Björk, M. Borgström, K. Deppert, K. Dick, A. Hansen, T. Mårtensson, N. Panev, A. Persson, et al., Physica E (Amsterdam) 25, 313 (2004).
[28] P. Kroghstrup, J. Yamasaki, C. Sorensen, E. Johnson, J. Wagner, R. Pennington, M. Aagesen, N. Tanaka, and J. Nygård, Nano letters 9, 3689 (2009).
[29] A. Wacker, Phys. Rev. B 66, 085326 (2002).
[30] F. Banit, S. C. Lee, A. Knorr, and A. Wacker, Appl. Phys. Lett. 86, 041108 (2005).
[31] D. Burghoff, C. W. I. Chan, Q. Hu, and J. L. Reno, Appl. Phys. Lett. 100 (2012).
[32] S. C. Lee, F. Banit, M. Woerner, and A. Wacker, Phys. Rev. B 73, 245320 (2006).