Nonequilibrium Green's Functions Theory for Intersubband Optics

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Intersubband transition based devices like the quantum cascade laser (qcl) are now important in the infrared spectral region, with interesting perspectives for applications in the THz regime. Recent detailed comparisons between theory and experiments have clearly demonstrated that many body effects are required to explain the intersubband optical absorption of quantum wells. However, the gain spectra of more complicated qcl structures have been explained relatively well without those effects. Our nonequilibrium Keldysh–Green's functions microscopic approach explains the apparent contradiction. We apply our theory to two limiting cases: qcl's, characterized by Wannier–Stark states and parabolic in-plane dispersion relations and coupled band quantum wells with strongly nonparabolic bandstructure and k-dependent transition dipole moments.

In the qcl structure, we demonstrate that the many-body effects depend essentially in the occupations of the subbands and on the detailed Coulomb matrix elements that describe the overlap of electronic wavefunctions. The combination of large population differences and occupation factors with large Coulomb matrix elements lead to strong Coulomb corrections on the THz region (absorption). However, in the mid-infra-red (gain) region, the Coulomb overlap integrals are small or the dominating gain transition. That explains the apparent contradiction, which requires the actual nonequilibrium distribution and realistic wavefunctions and Coulomb matrix elements, in contrast to simplifying approximations that are relatively successful for quantum wells, which fail in the more complex qcl superlattice scenario. Only transitions with TM polarization are possible.

In the multiple quantum well case, with conduction and valence subband contributions, the evolution of TM and TE modes is remarkably different and extra peaks can appear in the TE spectra due to the Coulomb interaction. Furthermore weak, but possibly resolvable conduction band contributions can be found in the TE spectra and their strength is increased by a combination of bandcoupling and Coulomb corrections, also demonstrated here for the first time. Moreover, the spectral positions and broadening, number of peaks and their relative oscillator strengths of the spectra calculated with and without Coulomb effects are radically different, further highlighting the relevance of our calculations

In summary, our fully quantum mechanical microscopic modeling of transport and optics of quantum cascade lasers demonstrates how to control the overall strength of Coulomb corrections by modifying the wavefunction overlap and thus the Coulomb matrix elements by means of an external bias. Our equilibrium calculations for nonparabolic subband quantum wells demonstrate strong interplays between bandstrcuture and many-body effects that can be relevant for the predictive simulations of possible new devices based on both conduction and valence subband transitions. These result have been obtained in collaboration with Andreas Wacker (Lund) and Hans Wenzel (FBH Berlin).