Non-Equilibrium Green's Functions Basis in Multiband Models for Broken-Gap Antimonide-Based Tunneling Devices

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Interband cascade lasers (ICLs) and detectors have shown promising properties for mid-infrared gas sensing applications. However, some of the performance degradations cannot be explained by known principles, particularly for longer wavelengths, in which the gas molecules relevant for medical and industrial purposes have their vibrational modes [1]. A rigorous theoretical modelling of the tunneling carrier transport, including the coupling of the conduction and valence bands, is desired for optimization of this class of devices.

The dynamics of electrons and holes in the ICL active region involve tunneling through potential barriers and their recombination (generation). Carriers in small- or closed-bandgap semiconductor heterostructures can be described by multiband models of the Schrödinger equation such as the 8-band $\mathbf{k}\cdot\mathbf{p}$ method (Fig. 1).

Two-point Green's functions (GFs) enable evaluation of the statistical average of time-dependent physical quantities since the expectation value of a product of field operators equals the sum of all pairwise contractions (Wick's theorem). The non-equilibrium Green's function (NEGF) formalism allows to include scattering mechanisms in devices under steady-state operation without relying on phenomenological parameters.

NEGF simulation of dissipative carrier transport using the 8-band model has been addressed recently [2]. The bottleneck is the numerical load caused by an increased number of basis states, required by the presence of the non-negligible interband coupling. The size of the problem can be reduced by switching the basis from the full real space grid [3] to a selected set of relevant states in the nanostructure such as the Wannier function basis [4], [5], [6].

Here, we present our extension of our NEGF solver nextnano.NEGF from intersubband to interband tunneling devices, with a focus on the basis functions of the GFs. We discuss how to capture the in-plane wavevector dependence, the influence of the interband coupling, and how to obtain the basis functions well describing the actual quasiparticles of the system, while minimizing the numerical overhead required in the following NEGF self-consistent loop.

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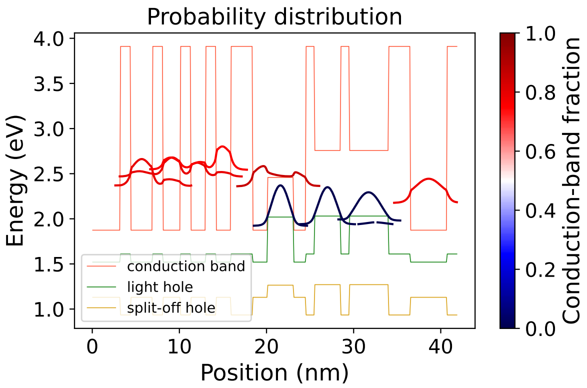

Fig. 1. Carrier probability distribution of lasing states (center), electron injector (left) and hole injector (right) in an interband cascade laser of Ref. [7] simulated by the 8-band $\mathbf{k} \cdot \mathbf{p}$ solver of the nextnano.NEGF. The color scheme of the wavefunctions signifies the fraction of the conduction-band components in the solutions.

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