Wigner Function Approach to Quantum Transport in QCLs

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Quantum cascade lasers (QCLs) are semiconductor heterostructures where lasing is achieved using transitions between localized quantum states. QCLs have received a considerable amount of attention ever since their first experimental realization in 1994 [1] and a wide range of modeling techniques, at varying degrees of approximation, have been employed to simulate electron transport in these structures [2], [3], [4], [5], [6]. A popular technique is to assume transport is semiclassical, due to scattering between quasi-bound states, with the rates calculated using Fermi's golden rule [3], [4]. Such an approximation is valid as long as transport is mostly incoherent. However, in THz QCLs, coherent transport and dephasing play important roles and have to be included [7]. Here, we demonstrate that the Wigner function formalism can accurately describe the effects of coherence and dephasing in THz QCLs, while avoiding the computational requirements of approaches using nonequilibrium Green's functions (NEGF) [5].

We solve the Wigner-Boltzmann transport equation (WBTE) using a particle-based numerical method [8], [9] where periodic boundary conditions are easily implemented. This approach is valid as long as the electron coherence length is shorter than the simulation domain. One of the advantages of this method is that the computational burden scales linearly with the system length. This is because the Wigner function $f(z, k)$ is defined in phase space, so doubling the system length only doubles the number of needed mesh points (and particle number) in the z direction. This is in contrast to density matrix approaches where doubling the system size results in a 4-fold increase due to the density matrix $\rho(z_1, z_2)$ dependence on two positions.

To demonstrate the validity of the Wigner function approach, we simulated a THz frequency QCL from Ref. [10], where lasing at a frequency of 1.8 THz was obtained for temperatures up to 168 K. Figure 1 shows the calculated conduction band profile, which is obtained from the WBTE simulation coupled with Poisson's equation. Also shown are the relevant subbands and their occupation at the design electric field of 15 kV/cm. From the figure we can see that our results predict a relative occupation $n_5/n_4 \simeq 1.64$, where n_5 (n_4) is the occupation of the upper (lower) lasing level. The results are consistent with the device achieving lasing at the design electric field of 15 kV/cm.

Figure 2 shows the calculated current density vs electric field for lattice temperature in the range 50-300 K. At low temperatures, the relationship between current density and electric field is highly non-linear with a plateau around 7 kV/cm and an NDR region around 13 kV/cm. However, at room temperature, the fine features are nearly washed out due to enhanced electron-phonon scattering, and the current vs field relationship is almost linear.

Figure 3 shows the steady-state Wigner function for different values of the applied electric field for a lattice temperature of 50 K. At zero field, electrons mostly occupy the ground state in the widest well and coupling between adjacent stages is low. For intermediate field strength (7.5 kV/cm), electrons also occupy the narrower wells and transport can be described as coupling between ground states in individual wells. At a higher field (15.0 kV/cm) significant delocalization occurs and states that are delocalized over multipe wells are occupied. The region around $k = 0$ in which the Wigner function has negative values are signs of high occupation of states that are delocalized between two or more wells, such as the upper and lower lasing level shown in Fig. 1.

We have demonstrated that the Wigner function

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formalism can be used to efficiently model electron transport in THz frequency QCLs. Effects of coherence and dephasing due to scattering are important in such devices and are included in our method. We were able to calculate microscopic quantities such as occupation of lasing states, which is crucial in QCL device design.

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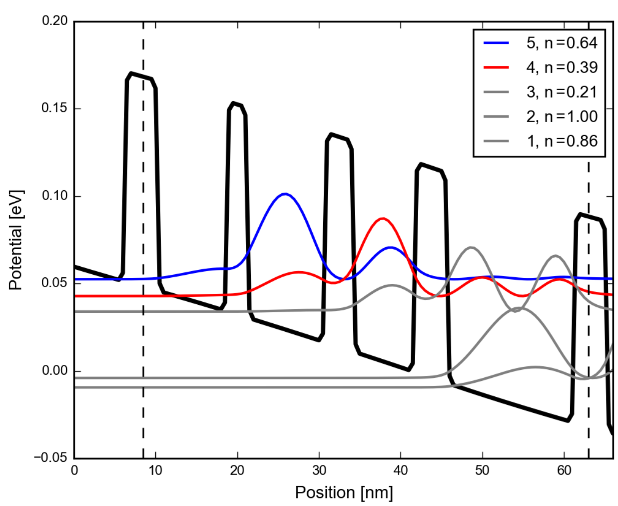

Fig. 1. Conduction band (thick black) along with the relevant subbands and their relative occupation (occupations are normalized such that the highest occupation is one) for the THz QCL structure from Kumar *et al.* [10]. The radiative transition is between subbands 5 and 4. Vertical dashed lines denote the extent of a single stage, which has a length of 54.5 nm.

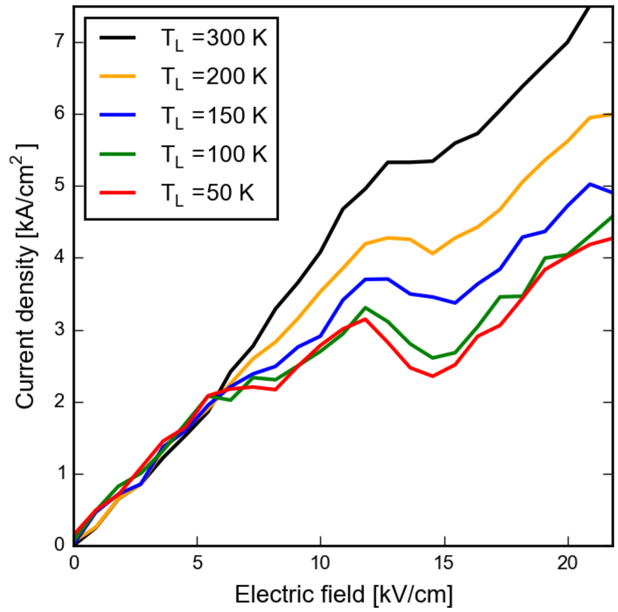

Fig. 2. Current density vs electric field for different lattice temperatures for the THz QCL structure from Kumar *et al.* [10].

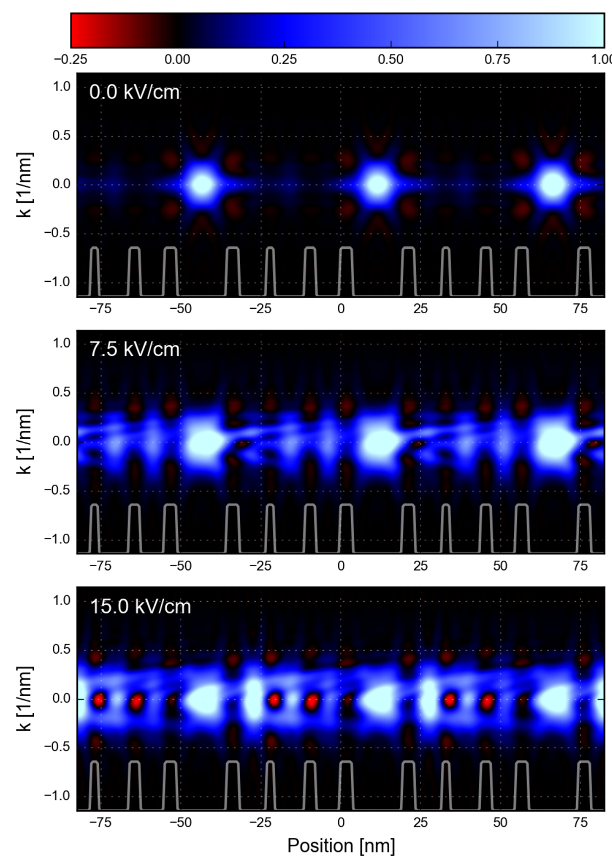

Fig. 3. The steady-state Wigner function for zero electric field (top), 7.5 kV/cm (middle), and 15.0 kV/cm (bottom) for the THz QCL structure from Kumar *et al.* [10]. Potential barriers are shown in white. The simulation domain is three stages, with a total length of 163.5 nm.