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Fourier transform-based scattering-rate method for self-consistent simulations of carrier transport in semiconductor heterostructures

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We present a self-consistent model for carrier transport in periodic semiconductor heterostructures completely formulated in the Fourier domain. In addition to the Hamiltonian for the layer system, all expressions for the scattering rates, the applied electric field, and the carrier distribution are treated in reciprocal space. In particular, for slowly converging cases of the self-consistent solution of the Schrödinger and Poisson equations, numerous transformations between real and reciprocal space during the iterations can be avoided by using the presented method, which results in a significant reduction of computation time. Therefore, it is a promising tool for the simulation and efficient design of complex heterostructures such as terahertz quantum-cascade lasers. © 2015 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4918671]

I. INTRODUCTION

The progress in semiconductor science and technology, in particular, the high-quality growth of complex planar heterostructures with more than one thousand layers, has allowed for the development of novel devices such as quantum-cascade lasers (QCLs). In the last decade, QCLs for the terahertz (THz) spectral region have been demonstrated to be promising light sources for applications in the field of THz imaging as well as absorption spectroscopy. In addition, THz QCLs have been demonstrated as local oscillators in heterodyne receivers. In many cases, the THz QCLs have to simultaneously fulfill an entire set of specifications with respect to lasing frequency, operating temperature, optical output power, and pumping power for a single device. Therefore, a model which can be implemented as a design tool for THz QCLs has to combine sufficient predictability with manageable computational costs. This is of particular importance for so-called hybrid designs with about ten quantum wells per period and an accordingly large number of states which have to be taken into account.

Carrier transport in semiconductor heterostructures can be simulated at various levels of complexity and predictability. Among these models, scattering-rate approaches, ensemble Monte Carlo methods, and non-equilibrium Green’s function formalisms are often used. For the design of complex structures such as THz QCLs, scattering-rate approaches taking into account only the occupation numbers or simplified density matrix methods are preferred since these approaches allow for sufficient accuracy compared to the experimental reproducibility of nominally identical structures with reasonable numerical effort. In order to adequately describe the effects of resonant coupling in complex structures, self-consistently calculated scattering rates, which are obtained from the actual wave functions of the states for each parameter set, have to be used rather than constant scattering rates determined before the self-consistent routine.

For the self-consistent determination of the carrier distribution and transport in the framework of a rate equation system or a simplified density matrix approach, first the Schrödinger equation is solved. Then, the carrier distribution is determined according to the transport model, which induces an additional potential so that the Schrödinger equation is solved again for a corrected potential and so forth. After successful convergence, which may depend on the total carrier (doping) density of the structure, the current density, and optical gain are determined. For current-voltage curves, this procedure has to be repeated for all values of the applied field strengths. In order to keep the computation time minimal, the fixed components of the Hamiltonian, i.e., the potential as defined by the layer system, should be determined once for all steps, while the potential caused by the applied electrical field is calculated once for each data point. For each loop of the self-consistent procedure, the Schrödinger equation is solved, the (generalized) scattering rates are calculated, and the carrier distribution as well as the Coulomb potential obtained by the solution of the Poisson equation is determined. Therefore, an efficient method for the solution of the Schrödinger equation and the rate equation system as well as the fast determination of the potential corrections is essential for minimal computational times. A schematic flow chart of the presented self-consistent model is shown in Fig. 1. In addition to the requirements for the use as a design tool, the minimization of the computational effort is also a prerequisite for the expansion of the model into a full density matrix approach in order to include coherent effects in the transport properties or to develop three-dimensional models, which allow for the investigation of lateral potential fluctuations.

While widely used approaches to solve the Schrödinger equation for QCLs focus on transfer matrix or finite difference methods, also Fourier transform-based methods were developed for quantum wells, superlattices, and quantum dots. The effective-mass approximations used in these works range from the Ben Daniel-Duke Hamiltonian to multiple-band kp models. For self-consistent calculations, also the Poisson equation has been expanded into plane-waves so that a compact system of the coupled Schrödinger and Poisson equations could be established. The Fourier transform methods allow for efficient numerical procedures and are expected to be powerful tools for the

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simulation of complex semiconductor heterostructures. We show that all components of the model can solely be formulated in the Fourier domain leading to a significant reduction of the computation time by about one order of magnitude.

II. FORMULATION OF THE HAMILTONIAN FOR THE FOURIER DOMAIN

We start from a two-band pseudo $k \cdot p$ model in order to take into account an energy-dependent effective mass

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \psi_1(z) \\ \psi_2(z) \end{pmatrix} = E \begin{pmatrix} \psi_1(z) \\ \psi_2(z) \end{pmatrix},$$

(1)

with $H_{11} = V(z), H_{12} = H_{21}, H_{22} = -\frac{\mu_0(z)}{\gamma(z)} + V(z) = -\frac{\mu_0(z)}{\gamma(z)} + H_{11}, V(z) = V_{\text{struc}}(z) + V_{\text{dop}}(z) + V_{\text{app}}(z) + V_{\text{elect}}(z)$ denotes the total potential profile in the $z$-direction for the electrons resulting from the layer structure, the positively charged dopants, the applied electrical field, and the Coulomb potential due to the electron distribution, respectively. Furthermore, $\mu_0$ denotes the free electron mass, $\mu_0(z)$ the effective electron mass in units of $\mu_0$ at the conduction band edge, $\gamma(z)$ the non-parabolicity parameter in units of $m_0$ per eV, and $\hbar$ Planck's constant. We expand $\psi_1(z)$ and $\psi_2(z)$ into Fourier series $\psi_a(z) = \sum_j \lambda_{a,j} \beta_j$ with $a = 1, 2$ and $\beta_j = \frac{1}{\sqrt{2\pi}} e^{2\pi i j z},$ where $i$ denotes the imaginary unit, $j$ the index of the Fourier component, and $L$ the length of the simulation cell. Equation (1) can now be written as

$$\begin{pmatrix} H_{11} \sum_j \lambda_{1,j} \beta_j \\ H_{21} \sum_j \lambda_{1,j} \beta_j \\ H_{21} \sum_j \lambda_{1,j} \beta_j \\ H_{22} \sum_j \lambda_{2,j} \beta_j \end{pmatrix} = E \begin{pmatrix} \sum_j \lambda_{1,j} \beta_j \\ \sum_j \lambda_{1,j} \beta_j \\ \sum_j \lambda_{1,j} \beta_j \\ \sum_j \lambda_{2,j} \beta_j \end{pmatrix}.$$

(2)

Multiplying both sides from the left with

$$\begin{pmatrix} \beta_m^* \\ 0 \\ 0 \\ \beta_m^* \end{pmatrix}$$

(3)

and integrating over $z$ leads, due to the orthonormality problem for $\lambda_{a,j}$

$$\sum_j |\beta_m| |H_{11}| |\lambda_{1,j}| + \sum_j |\beta_m| |H_{12}| |\lambda_{2,j}| + \sum_j |\beta_m| |H_{21}| |\lambda_{1,j}| + \sum_j |\beta_m| |H_{22}| |\lambda_{2,j}| = E |\lambda_{1,m}|$$

(4)

or

$$\sum_a \sum_j H_{b,m,j} \lambda_{a,j} = E \lambda_{b,m}.$$

(5)

with $H_{b,m,j} = \langle \beta_b | H_{b,a} | \beta_j \rangle$ and $b = 1, 2$, which can be easily solved using standard numerical packages leading to a set of eigenvalues $E_n$ and eigenfunctions $(\lambda_{n,1}, \lambda_{n,2})$ with their components $\lambda_{n,1,m}$ and $\lambda_{n,2,m}$.

While $H_{1m,1j}$ and $H_{2m,1j}$ are fixed and can be calculated at the beginning of the computation, the diagonal components of the Hamiltonian $H_{1m,1j}$ and $H_{2m,2j}$ contain the complete potential $V(z)$. Therefore, we may separate the diagonal components $H_{1m,1j}$ and $H_{2m,2j} = H_{1m,1j} + H_{2m,2j}^\text{app}$, with $H_{2m,2j}^\text{app} = \langle \beta_m | - \frac{\mu_0(z)}{\gamma(z)} | \beta_j \rangle$ into constant components and components depending on the applied field and the carrier distribution according to $H_{1m,1j} = H_{1m,1j}^\text{struc} + H_{1m,1j}^\text{dop} + H_{1m,1j}^\text{app} + H_{1m,1j}^\text{elect}$.

A. Constant components of the Hamiltonian

The components related to the layer sequence can be straightforwardly calculated if we assume a piecewise constant potential $V_{\text{struc}}(z) = \sum_{p=1}^{P_{\text{tot}}} V_p \Theta(z - z_p) \Theta(z_p + \Delta_p - z)$ expressed in terms of the Heaviside step function $\Theta$ for a structure with $P_{\text{tot}}$ layers and $V_p$ denoting the (constant) potential, $\Delta_p$ the thickness, and $z_p$ the position of the left boundary of the $p$th layer.

$$H_{1m,1j}^\text{struc} = \frac{1}{L} \int_0^L e^{-2\pi i n z} V_{\text{struc}}(z) e^{2\pi i j z} dz$$

$$= \begin{cases} \frac{1}{L} \sum_{p=1}^{P_{\text{tot}}} V_p \Delta_p & \text{for } j = m \\ \frac{1}{2\pi i (j - m)} \sum_{p=1}^{P_{\text{tot}}} V_p \left[ e^{2\pi i n \Delta_p + \Delta_p} - e^{2\pi i n \Delta_p} \right] & \text{for } j \neq m. \end{cases}$$

(6)
For the case of a periodic structure with \( P \) layers per period, the summation needs to be carried out only for one period, and the result has to be multiplied by \( N_{\text{per}} \) (the number of periods) if \( j = m \) or by a factor

\[
\Phi_{\text{per}}^{jm} = \sum_{p=1}^{N_{\text{per}}} e^{2\pi i (j-m)p \xi_p},
\]

for \( j \neq m \). For a more realistic description of the composition profile, a sigmoidal interface grading, which can be approximated by a Gaussian function in reciprocal space, can be taken into account.\(^{25}\) By multiplying the components of the potential with

\[
\Phi_{\text{sigm}}^{jm} = e^{-\frac{1}{2} \left(\frac{z - \xi_p}{\Delta z}\right)^2},
\]

we obtain

\[
H_{1m,1j}^{\text{struc}} = \begin{cases} 
\frac{N_{\text{per}}}{L} \sum_{p=1}^{P} V_p \Delta_p & \quad \text{for } j = m \\
\frac{\Phi_{\text{per}}^{jm} \Phi_{\text{sigm}}^{jm}}{2\pi i (j-m)} \sum_{p=1}^{P} V_p \left(e^{2\pi i \xi_p (\xi_p + \Delta_p)} - e^{2\pi i \xi_p \Delta_p}\right) & \quad \text{for } j \neq m,
\end{cases}
\]

for an interface parameter \( L_c \). According to Ref. 26, the interface width is about 4.4\( L_c \). Similarly, the Fourier components of the other structure-dependent components are given by

\[
H_{2m,2j}^{\text{struc}} = \begin{cases} 
\frac{N_{\text{per}}}{L} \sum_{p=1}^{P} \tilde{\gamma}_p \Delta_p & \quad \text{for } j = m \\
\frac{\Phi_{\text{per}}^{jm} \Phi_{\text{sigm}}^{jm}}{2\pi i (j-m)} \sum_{p=1}^{P} \tilde{\gamma}_p \left(e^{2\pi i \xi_p (\xi_p + \Delta_p)} - e^{2\pi i \xi_p \Delta_p}\right) & \quad \text{for } j \neq m,
\end{cases}
\]

with \( \mu_{0,p} \) denoting the effective mass and \( \tilde{\gamma}_p \) the non-parabolicity parameter in the \( p \)th layer of the period and

\[
H_{1m,2j} = H_{2m,1j} = \begin{cases} 
-\frac{2\pi \hbar}{\sqrt{2m_0} L} \sum_{p=1}^{P} \frac{1}{\sqrt{\tilde{\gamma}_p}} \Delta_p & \quad \text{for } j = m \\
\frac{i \hbar \Phi_{\text{per}}^{jm} \Phi_{\text{sigm}}^{jm}}{\sqrt{2m_0} (j-m)} L \sum_{p=1}^{P} \frac{1}{\sqrt{\tilde{\gamma}_p}} \left(e^{2\pi i \xi_p (\xi_p + \Delta_p)} - e^{2\pi i \xi_p \Delta_p}\right) & \quad \text{for } j \neq m,
\end{cases}
\]

In order to determine the component of the Hamiltonian related to the positively charged doping, we use the Poisson equation in the \( z \) direction for a given doping density \( \rho_{\text{dop}}(z) \)

\[
\frac{\partial^2}{\partial z^2} V_{\text{dop}}(z) = \frac{e}{\varepsilon_0 \varepsilon_r} \rho_{\text{dop}}(z),
\]

(10)

in terms of the respective Fourier components (except for \( j = 0 \))

\[
V_{\text{dop},j} = -\frac{e}{\varepsilon_0 \varepsilon_r} \frac{L^2}{(2\pi)^2} \rho_{\text{dop},j},
\]

(11)

with \( \varepsilon_r \) denoting the relative permittivity, \( \varepsilon_0 \) the vacuum permittivity, and \( e \) the elementary charge. We set \( V_{\text{dop},0} = 0 \), to define the origin of the energy scale. Then, the elements of the Hamiltonian are

\[
H_{1m,1j}^{\text{dop}} = \frac{1}{L} \int_0^L e^{-2\pi i \xi_p \xi} V_{\text{dop}}(z) e^{2\pi i \xi z} dz
\]

\[
= \frac{1}{L} \int_0^L e^{-2\pi i \xi z} \sum_q V_{\text{dop},q} e^{2\pi i \xi q z} dz
\]

\[
= \sum_q V_{\text{dop},q} \frac{1}{L} \int_0^L e^{2\pi i \xi q z} dz = V_{\text{dop},(m-j)}
\]

\[
= -\frac{e}{\varepsilon_0 \varepsilon_r} \frac{L^2}{(2\pi)^2} \rho_{\text{dop},(m-j)},
\]

(12)

With

\[
\rho_{\text{dop},q} = \frac{1}{L} \int_0^L \rho_{\text{dop}}(z) e^{-2\pi i \xi z} dz,
\]

(13)

a piecewise constant doping density \( N_p \) in the \( p \)th layer leads to
Again, we may take into account a sigmoidal profile at the interface between doped and undoped regions by multiplying with $\Phi_{jm}^{\text{sigm}}$. We may assume the same interface parameter $L_i$ as for the composition profile or use a modified factor $\Phi_{jm}^{\text{sigm, dop}}$ for a specific $L_i^{\text{dop}}$.

**B. Components depending on the applied field**

For the simulation of current-voltage curves, the applied voltage, which leads to an additional linear potential drop $V_{\text{app}}(z) = Fz$ across the entire structure with $F$ denoting the applied voltage divided by the total thickness, has to be varied. The respective components of the Hamiltonian are

$$H_{1m,ij}^{\text{appl}} = \begin{cases} F L & \text{for } j = m \\ F \frac{L}{2 \pi i (j - m)} & \text{for } j \neq m \end{cases}$$

and have to be calculated once for each point of the curve.

**C. Components depending on the carrier distribution**

For the self-consistent procedure, the potential correction due to the charge distribution related to the carriers has to be determined for each loop. Based on an appropriate transport model, this potential is determined from the carrier distribution. Again, we start from the Poisson equation (11) for the Fourier domain using the carrier distribution according to

$$\rho_{\text{elec}}(z) = N_{\text{aver}} \sum_n \rho_{nn}(|\psi_{n,1}(z)|^2 + |\psi_{n,2}(z)|^2),$$

with $\rho_{nn}$ denoting the occupation number of the $n$th state and $N_{\text{aver}}$ the average volume density of carriers. The transformation into reciprocal space leads to

$$\rho_{\text{elec}, q} = \frac{1}{L} \int_0^L \rho_{\text{elec}}(z) e^{-2\pi i q z} dz$$

and

$$\rho_{\text{elec}, q} = \frac{1}{L} \int_0^L N_{\text{aver}} \sum_n \rho_{nn} \left(|\psi_{n,1}(z)|^2 + |\psi_{n,2}(z)|^2\right) e^{-2\pi i q z} dz$$

and

$$\rho_{\text{elec}, q} = \frac{1}{L} \sum_n \rho_{nn} \sum_{k} \left(\lambda_{n,1,k}^* z_{n,1,k} + \lambda_{n,2,k}^* z_{n,2,k}\right) e^{2\pi i q z}$$

for $j = m$

$$H_{1m,ij}^{\text{elec}} = \begin{cases} 0 & \text{for } j = m \\ N_{\text{aver}} e \frac{\Phi_{jm}^{\text{per}} L^2}{2 \pi i q} \sum_{n,k} \rho_{nn} \left(\lambda_{n,1,k}^* \lambda_{n,1,k+j} + \lambda_{n,2,k}^* \lambda_{n,2,k+j}\right) & \text{for } j \neq m \end{cases}$$

Again, we take into account only states belonging to one period of the system and expand the charge distribution to the entire periodic structure by multiplying with $\Phi_{jm}^{\text{per}}$.

**III. SCATTERING RATES FOR THE FOURIER DOMAIN**

In order to determine $\rho_{\text{elec}}$, the electron distribution has to be calculated, for instance, by using scattering-rate approaches or density matrix methods. A scattering-rate approach with scattering rates determined self-consistently from the actual wave functions for each iteration loop was shown to be sufficiently precise and efficient for the design of a THz QCL used as a local oscillator for a 4.745 THz heterodyne spectrometer and for the achievement of the highest operating temperatures of continuous-wave THz QCLs at 3 THz. For this model, the in-plane momentum of the electrons is neglected, and the scattering rates $T_{nm}$ are assumed to be proportional to the squared moduli of the dipole matrix elements $D_{nm} = \langle \psi_n(z) | z | \psi_m(z) \rangle$ of the respective transitions with an empirical factor which depends on the transition energy and is significantly larger than for the electron-photon interaction. In the framework of our model, we will finally formulate the dipole matrix elements in reciprocal space

$$D_{nm} = \frac{1}{L} \int_0^L \left[\psi_{n,1}(z) \psi_{m,1}(z) + \psi_{n,2}(z) \psi_{m,2}(z)\right] dz$$

and

$$D_{nm} = \frac{1}{L} \int_0^L \left(\lambda_{n,1,m}^* \lambda_{n,1,m+j} + \lambda_{n,2,m}^* \lambda_{n,2,m+j}\right) e^{2\pi i q z} dz$$

for $j = m$

$$D_{nm} = \frac{1}{L} \int_0^L \left(\lambda_{n,1,m}^* \lambda_{n,1,m+j} + \lambda_{n,2,m}^* \lambda_{n,2,m+j}\right) \left(2 \pi i (j - m) \right)$$

for $j \neq m$. (19)
This approximation is among the most straightforward ones in terms of Fourier representation for the scattering rates. For scattering of electrons at longitudinal optical phonons, for instance, the approximation using the dipole matrix element as the form factor of the interaction matrix element is appropriate for configurations in which only phonons with small wave vector contribute. Note, however, that this is still an approximation which may lead to much too low transition rates in cases with a vanishing dipole matrix element despite a finite overlap of the electron wave functions. Such a situation may occur, for instance, for a transition between states with the same parity in a single quantum well. In general, this approximation might become questionable as it neglects the in-plane degree of freedom and introduces the dipole-related parity rule. Furthermore, it is less suitable for elastic processes. In many cases, however, these restrictions do not dominate the results, in particular, for QCL structures with wave functions extending over more than one quantum well as shown in Ref. 23 for various design types. High-end THz QCLs, which fulfill an entire set of challenging specifications, can efficiently be developed by combining fast simulations for a large number of designs with empirical investigations of the devices. The trade-off between accuracy and computational efforts of the simulation, in particular, for the simulation of complex structures with many relevant states, has recently allowed for the development of the local oscillator\textsuperscript{6} for 4.745 THz and justifies such approximations at least for individual cases.

### IV. IMPLEMENTATION

The first iteration loop starts with the solution of the Schrödinger equation using either a homogeneous charge distribution or, for instance, in the case of current-voltage characteristics, the distribution obtained for the previously applied field strength. Then, relevant states are selected by (i) excluding states with too high energies, for instance, states above the barrier band edge, and (ii) taking into account only states within two periods in order to allow for scattering within a period and between neighboring periods. For an identification of equivalent states of neighboring periods, we verify the orthonormality condition between state $n$ of one period and state $\bar{n}$ shifted by the period length $L_{\text{per}}$ of the next period according to

\begin{equation}
\delta_{n\bar{n}} = \sum_{j} \left( \lambda_{n,1}^* \lambda_{\bar{n},1,j} + \lambda_{n,2}^* \lambda_{\bar{n},2,j} \right) e^{2\pi i q n / L_{\text{per}}},
\end{equation}

where $\epsilon$ denotes the computational accuracy. We write the rate equations,\textsuperscript{28} which represent the well known Boltzmann equation, in the form

\begin{equation}
\frac{d\rho_{n+np}(n'+np)}{dt} = \sum_{n=1}^{n_p} \sum_{q=1}^{n_p} \left( T_{n+np}(n+qp) \rho_{n+qp}(n+qp) - T_{n+np}(n'+qp) \rho_{n'+qp}(n'+qp) \right).
\end{equation}

$T_{n+qp}(n'+qp)$ denotes the rate for scattering from the $n'$th state of the $p$th period to the $n$th state of the $q$th period and $n_p$ the total number of states in each period. The periodicity leads to $\rho_{n+np}(n+qp) = \rho_{nm}$ and $\rho_{n'+np}(n'+qp) = \rho_{n'm'}$, while $T_{n+np}(n'+qp)$ $\neq T_{n'+np}$ if $p \neq q$. Furthermore, for $|p-q| > 1$, we assume $T_{n+qp}(n'+qp) = 0$. Obviously

\begin{align*}
T_{n+np}(n'+np) &= T_{nm'}, \\
T_{n+np}(n'+np) &= T_{n'm}, \\
T_{n+np}(n'+np) &= T_{n(n'+np)}. 
\end{align*}

Therefore, we may simplify the rate equations for the steady state to

\begin{equation}
0 = \frac{d\rho_{n'm'}}{dt} = \sum_{n=1}^{n_p} \sum_{q=1}^{n_p} \left( T_{n+np}(n+qp) \rho_{nm} - T_{n+np}(n'+qp) \rho_{n'm'} \right)
= \sum_{n=1}^{n_p} \left( [T_{n+np}(n+np) + T_{n'+np}(n+np)] \rho_{nm} - [T_{n+np}(n+np) + T_{n'+np}(n+np)] \rho_{n'm'} \right).
\end{equation}

and need to calculate the scattering rates $T_{nm'}$ only for transitions between those states $n$ and $n'$ which are located in two adjacent periods. The neutrality condition requires the additional equation

\begin{equation}
1 = \sum_{n} \rho_{nn},
\end{equation}

so that we have to modify, for example, the first equation ($n' = 1$) of the above system to

\begin{equation}
1 = \sum_{n=1}^{n_p} \left( [1 + T_{1+np}(1)] + T_{1+np}(n+np) \rho_{nn} - [T_{1+np}(1) + T_{1+np}(n+np)] \rho_{n1} \right).
\end{equation}

The occupation numbers obtained by solving this inhomogeneous system of linear equations is used for the determination of $H_{1m1j}^{\text{elec}}$ according to Eq. (18). After sufficient convergence of the iteration loop, the current density\textsuperscript{29}

\begin{equation}
J = eN_{\text{aver}} \sum_{n} T_{n+np} \rho_{mn} (D_{nn'} - D_{nn})
\end{equation}

and the optical gain\textsuperscript{23}

\begin{equation}
G(\omega) = \frac{\omega \pi e^2}{cnBqL_{\text{per}}} \sum_{n,n'} \left( N_{n} - N_{n'} \right) |D_{nn'}|^2 \left( E_{nn'} \right),
\end{equation}
with a Lorentzian line shape

\[ L_{nn'} = \frac{\Gamma_{nn'}}{2\pi \left( \hbar \omega - E_{nn'} \right)^2 + \left( \Gamma_{nn'}/2 \right)^2}, \]  

(27)

using \( \Gamma_{nn'} = \Gamma_n + \Gamma_{n'} \) and \( E_{nn'} = E_n - E_{n'} \) can be determined. The level broadening is determined by

\[ \Gamma_n = \hbar \sum_{n'} T_{n'n}. \]  

(28)

Inhomogeneous broadening may be taken into account by adding a value of a few meV. \( E_n \) and \( \nu = \omega/(2\pi) \) denote the energy of state \( n \) and the photon frequency, respectively. We use \( n_B = \sqrt{13} \) for the background refractive index at THz frequencies. Finally, the self-consistent potential, e.g., as shown in Figs. 2–4 of Ref. 25, can be calculated by the respective back transformation. Using the relationship between the Fourier components of the Hamiltonian and the potential \( H_{1m,1j} = V_{m-j} \), we obtain

\[ V(z) = \sum_{m-j} H_{1m,1j} e^{2\pi i m z / \lambda}. \]  

(29)

V. RESULTS

Figure 2 shows a comparison of the current density-applied electric field strength characteristics calculated for sample B1 of Ref. 6 using the Fourier domain method as well as using the real-space method according to Ref. 23. The data coincide rather well, which confirms the mathematical equivalence of the two methods. The deviations are attributed to the convergence behavior during the self-consistent procedure, which depends sensitively on the actual initial charge distribution and small numerical differences. Nevertheless, these deviations are smaller than typical fluctuations in the current levels of nominally identical lasers processed from different wafers. The most important achievement of the Fourier domain method is to reduce the simulation time by about one order of magnitude compared to the previous real-space method.

In a similar way, the calculated gain spectra obtained by using the two methods agree quite well as shown in Fig. 3. Both gain maps exhibit their gain maxima at similar frequencies with similar maximum values. The gain spectra display the same red shift with increasing applied electrical field strength, and the behavior of the corresponding lasers is well reproduced. The offset of about 0.3 THz between the position of the gain maximum and the actual lasing frequency is again on the same order of magnitude as the typical deviations of lasing energies between nominally identical lasers obtained from wafers grown at different times.

Figure 4 shows the current density-applied electric field strength characteristics calculated for sample B1 of Ref. 6 using Fourier components \( j, m = -75 \) to 75 with a step width for the applied electrical field strength of 0.1 kV/cm. The

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**FIG. 2.** Current density-applied field strength characteristics (upper panel) for sample B1 of Ref. 6 calculated using the Fourier domain method (dots) compared with the respective curve obtained from the previous real-space method (diamonds). The lower panel depicts a schematic view of about one period of the subband structure (conduction band edge and squared moduli of the wave functions) at an electric field strength of 5 kV/cm. For clarity, we show only the lowest states. The thick (blue) lines depict the laser levels.

**FIG. 3.** Calculated gain maps for sample B1 of Ref. 6 using the real-space method (top panel) as well as the Fourier domain method (2nd panel from top) compared to corresponding experimental lasing spectra (bottom panel). The third panel shows the gain spectra obtained by the two methods for 4.8 kV/cm. The experimental details are given in Ref. 6.
simulated curve agrees well with the measured characteristics below the onset of negative differential conductance. For higher field strengths, the experimental values are larger than the simulated ones, which we attribute to increasing leakage currents. Due to the formation of electric field domains, the region of negative differential conductance is not accessible by measurements. For this example, we obtained the partial computation times $T_{\text{const}} = 0.27$ s, $T_{\text{sch}} = 0.75$ s, $T_{\text{scatter}} = 0.51$ s, and $T_{\text{coul}} = 0.08$ s, i.e., the total time for one iteration loop is about 1.4 s. For the calculation of the wave functions in real space with a grid width of 0.2 nm over the entire simulation cell of 4 QCL periods, we obtain $T_{\text{WF}} = 5.51$ s for each field strength. If the scattering rates and carrier distribution would be determined from the real-space wave functions for each iteration loop, then the rather large value for $T_{\text{WF}}$ would have to be multiplied by the number of loops, which would increase the computation time significantly. Finally, typical computation times for the current density-applied field strength characteristics and gain spectra for 100 values of the field strength are about 50 min for the real-space model and about 5 min for the Fourier-based model using a typical workstation configuration.

A striking feature is the discontinuous appearance of the curves in Fig. 2, which seems to be a result of numerical inaccuracy. Therefore, we repeated the calculation with a step width of 0.002 kV/cm for an up and a down sweep. The sweep direction for the simulation is defined by the initial charge distribution used for the self-consistent procedure. For the case of an up (down) sweep, we use the calculated charge distribution for the adjacent lower (higher) field strength. Figure 5 reveals that most of the original data points follow the fine structure of the high-resolution up-sweep curve. The fine structure may be in part attributed to an overestimation of coupling between remote states, which is well known for rate equation models, or to artifacts due to the dipole approximation for the scattering rates. Even the high-resolution characteristic still exhibits a discontinuous appearance for some data points. Furthermore, we observe a significant bistability above the onset of negative differential conductance in the range from 7 to 10 kV/cm as well as several smaller regions, e.g., at about 4 kV/cm, where the data for both sweep directions clearly differ. The calculated hysteresis, which we attribute to multiple solutions of the Schrödinger-Poisson equation system, and the large jumps of the current density, e.g., at about 2.8, 3.4, or 4.3 kV/cm, are not observed in experiments. Therefore, we believe that the simulation of the current density-applied field strength characteristics with lower resolution and subsequent smoothing as demonstrated in Fig. 4 together with the calculation of the optical gain maps as shown in Fig. 3 are usually the appropriate way for an efficient and fast design of complex devices such as THz QCLs. If a more refined determination of the transport properties is required, the discussed model may be improved by replacing the classical rate equation system [Eqs. (21)–(24)] by the respective system for the complete density matrix and/or by using realistic scattering rates. In order to keep the computation time manageable, the respective generalized scattering rates have to be formulated in the Fourier domain. However, for the design of THz QCLs, the present status of experimental reproducibility of nominally identical structures suggests that in most cases the use of the discussed semiclassical method is still appropriate.

**VI. CONCLUSIONS**

We demonstrated a semiclassical transport model based on the self-consistent solution of the Schrödinger and Poisson equations in the framework of a scattering-rate approach. The expressions were formulated completely in the Fourier domain. The achieved fast simulation of the transport properties allows for the analysis of high-resolution current density-field strength characteristics as well as for an efficient design of complex heterostructures such as THz QCLs. This approach may be the starting point for the development of a full density matrix model with manageable computational effort.
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3. B. S. Williams, Nat. Photonics 1, 517 (2007), and references therein.
30. For details, see www.originlab.com (→ signal processing → smoothing/FFT filter).
32. We used one core of a 24 × Opteron 6176 processor at 2.3 GHz with 64 GB RAM.
33. We used 8 cores in parallel of a 24 × Opteron 6176 processor at 2.3 GHz with 64 GB RAM.