Optoelectronic Device Simulations Based on Macroscopic Maxwell–Bloch Equations

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Due to their intuitiveness, flexibility, and relative numerical efficiency, the macroscopic Maxwell–Bloch (MB) equations are a widely used semiclassical and semi-phenomenological model to describe optical propagation and coherent light–matter interaction in media consisting of discrete-level quantum systems. This review focuses on the application of this model to advanced optoelectronic devices, such as quantum cascade and quantum dot lasers. The Bloch equations are here treated as a density matrix model for driven quantum systems with two or multiple discrete energy levels, where dissipation is included by Lindblad terms. Furthermore, the 1D MB equations for semiconductor waveguide structures and optical fibers are rigorously derived. Special analytical solutions and suitable numerical methods are presented. Due to the importance of the MB equations in computational electrodynamics, an emphasis is placed on the comparison of different numerical schemes, both with and without the rotating wave approximation. The implementation of additional effects which can become relevant in semiconductor structures, such as spatial hole burning, inhomogeneous broadening, and local-field corrections, is discussed. Finally, links to microscopic models and suitable extensions of the Lindblad formalism are briefly addressed.

1. Introduction

Due to advancements in nanotechnology, structuring in the nanometer range is meanwhile routinely exploited in electronics and photonics. For example, in optoelectronic devices such as semiconductor optical amplifiers and lasers, quantum confinement is widely used to concentrate the carriers in certain energy states, yielding improved wall-plug efficiencies and higher output powers. As a further effect, the wavelength can be tuned by changing the size of the confinement structure. On a commercial basis, mostly 1D confinement is used in the form of quantum well structures, which are fabricated based on deposition of nanometer-thin semiconductor layers of different compositions. In such structures, a quantum well is formed by a layer consisting of a lower bandgap material than the adjacent layers, which restricts the free electron motion in that layer to the in-plane directions and gives rise to quantized energy states in growth direction. As a consequence of the further restriction of the energy spectrum and the even stronger carrier localization, additional improvement can be expected from 2D or 3D confinement, resulting in quantum wire/dash and quantum dot (QD) structures, respectively. Indeed, QD\(^{1–3}\) and quantum dash\(^{4}\) lasers and laser amplifiers have been shown to exhibit excellent characteristics. In Figure 1, the formation of quantized states in quantum wells, wires, and dots is schematically illustrated. The term quantum dash refers to an elongated nanostructure, that is, some kind of short quantum wire. By contrast, the term nanowire does not necessarily indicate strong quantum confinement. For example, in nanowire lasers, the nanowire geometry typically serves as a single-mode optical waveguide resonator, while the active region is based on a heterostructure or quantum well, as in a conventional laser diode.\(^{5,6}\)

Semiconductor optoelectronic devices usually rely on electron–hole recombination, that is, optical transitions between conduction and valence band states. The associated resonance wavelength is largely determined by the semiconductor bandgap, which establishes a lower bound on the transition energy. Thus, the coverage of a certain spectral region depends on the existence of suitable semiconductor materials, which for example restricts the availability of practical optoelectronic sources and detectors in the mid-infrared and terahertz regions. An alternative concept is based on intersubband devices, which employ so-called intersubband transitions between quantized energy states in the conduction (or, in some cases, valence) band of a nanostructure, and thus allow quantum engineering of the transition wavelength independent of the bandgap. Quantum well devices based on this concept include quantum cascade lasers,\(^7\) quantum cascade detectors,\(^8,9\) and quantum well infrared photodetectors.\(^10\) Furthermore, intersubband transitions are used for QD infrared photodetectors.\(^11–13\)

Along with quantum confinement, quantum coherent effects are also found to be increasingly relevant for modern optoelectronic devices. Such effects result from the coherent light–matter interaction, which requires that the states involved in the optical
transition maintain a well-defined phase relationship over a significant time. The coherent interaction manifests itself in so-called Rabi flopping\cite{14}, that is, carrier population oscillations between the states, which are driven by the optical field. The resulting carrier dynamics couples back to the optical field via the polarization, thus also affecting the propagating optical waveform. Besides being an essential prerequisite for the emerging field of quantum information technology\cite{15}, quantum coherence plays an increasingly important role for modern optoelectronic devices in general. Due to the strong interaction with the semiconductor environment, for example, in the form of phonon scattering and carrier–carrier interactions, this phase relationship tends to be quickly destroyed, which is commonly referred to as dephasing. However, under favorable conditions, signatures of Rabi oscillations have been observed in nanostructured optoelectronic systems and devices. These include quantum well structures\cite{16,17}, nanowire lasers\cite{8} quantum cascade lasers\cite{18}, and single QDs\cite{19,20} at cryogenic temperatures, as well as QD\cite{21,22} and quantum dash\cite{23} amplifiers at room temperature. Closely related is self-induced transparency\cite{24,25}, where Rabi flopping enables a special optical pulse form to propagate without being attenuated or disturbed. This phenomenon has meanwhile also been observed in semiconductor structures such as QD waveguides\cite{22,26} with potential applications such as the generation of ultrashort optical pulses in QD and quantum cascade lasers\cite{27–31}. Another effect that relies on quantum coherence is slow light propagation or even complete halting of light\cite{32–34} with possible applications such as optical buffers\cite{35}, imaging\cite{36,37} and quantum memory\cite{38}. This effect has meanwhile also been demonstrated in solid-state media, namely in doped crystals\cite{39,40}. The use of suitably engineered semiconductor structures would be especially attractive from a practical point of view\cite{41–43}. Furthermore, quantum interference, for example, in QD or intersubband quantum well systems, is an interesting candidate to realize all-optical switching.\cite{44,45} Due to the discrete energy level structure of QDs, semiconductor devices based thereupon are especially likely to be, at least in part, governed by coherence effects\cite{15}, although for QD ensembles the dephasing tends to be strong.\cite{21} The same applies to intersubband quantum well devices, where the levels close to the band edge have parallel dispersion relations, and thus the quantum dynamics resembles that of discrete-level systems.\cite{18} Especially in such devices, coherence effects can significantly influence the dynamic operation even for considerable dephasing.

Suitable theoretical models are required for an in-depth understanding of the often quite complex interplay of effects determining the dynamic device characteristics, as well as for quantitative simulation and systematic device optimization.
For the optoelectronic devices and structures discussed above, an adequate theoretical description must include the coherent carrier dynamics, incoherent processes such as scattering or spontaneous emission, as well as the interaction with the optical field. Our focus is here on the very widely used Maxwell–Bloch (MB) equations. The Bloch equations provide a compact model for the discrete-level carrier dynamics, which is described by the density matrix formalism. The coherent single-carrier dynamics is here modeled by the Hamiltonian of the quantum system, such as a QD, and also includes the interaction with a classical optical field. Effects beyond the single-electron quantum evolution are regarded as interaction with the environment in form of the semiconductor host, which gives rise to incoherent effects such as scattering with other carriers and phonons. The resulting dissipation in the quantum system is in the Bloch equations phenomenologically modeled by relaxation rate terms, which introduce dephasing and incoherent carrier transitions. The Bloch equations were first devised to describe the evolution of the nuclear magnetic moment in a magnetic field, and later on extended to a pair of levels in resonance with a classical optical field. The model is closed by coupling the Bloch equations to Maxwell’s equations, which describe the evolution of the classical optical field. This review paper is concerned with the resulting MB equations, where we go beyond the often applied two-level approximation by considering multiple, albeit discrete, energy levels. Furthermore, we root the phenomenological dissipation terms in the Lindblad formalism, which ensures physical behavior of the quantum system and allows for the construction of more general dissipation terms.

The MB equations offer a generic description of semiclassical light–matter interaction, which can be applied to different media such as semiconductor structures or gases. The focus of this review lies on semiconductor structures, which is reflected in the treatment of some specific issues, such as the concrete embodiment of Maxwell’s equations, or the inclusion of spatial hole burning in linear resonators. Independent of the modeled system, the main attractiveness of the MB equations lies in the relatively compact description of the carrier dynamics, which is helpful for providing intuitive insight into the device behavior and even allows for closed analytical solutions in some special cases. From a computational point of view, the Bloch equations are widely used in combination with electromagnetic simulations, for example, based on the finite-difference time-domain method, as a quantum model of the medium, replacing simpler classical descriptions such as the Lorentz model. Due to the relative compactness of the Bloch model, also computationally demanding 2D or 3D simulations can be carried out. Likewise, the MB equations enable systematic device optimizations over a large parameter range, as well as long-term simulations, for example, to investigate the steady-state laser dynamics. Another important advantage of the MB equations is that they can easily be adapted to specific problems by adding further effects, such as inhomogeneous broadening or local-field corrections.

Clearly, the Bloch equations constitute a compromise between accuracy and compactness of the model. A full microscopic treatment of light–matter interaction in a semiconductor, accounting for carrier–phonon and many-body Coulomb interactions as well as for free carrier motion in the unconfined directions, results in the so-called semiconductor MB equations. These do not require phenomenological input parameters, but the significantly increased model complexity usually restricts the modeling to one spatial dimension and short-term simulations. While the semiconductor MB equations are beyond the scope of this review, they can be used as a basis to derive macroscopic discrete-level MB equations with Lindblad dissipation and additional correction terms for specific semiconductor structures.

In detail, our paper is organized as follows: in Section 2, the density matrix formalism and Lindblad model are introduced, serving as a basis for the Bloch equations. These are treated in Section 3, which also includes a discussion of the widely used rotating wave approximation (RWA). In Section 4, the MB equations are introduced in full-wave treatment and invoking the RWA, along with the slowly varying amplitude approximation (SVAA) for the field propagation. Section 5 treats the reduction of the MB equations for semiconductor waveguide structures and optical fibers to a spatially 1D model, which is a widely used simplification. Section 6 deals with available analytical solutions for the Bloch and MB equations, while in Section 7, numerical methods for the MB equations are covered. Section 8 is dedicated to the inclusion of further effects, such as local-field corrections, inhomogeneous broadening, and noise. Section 9 deals with the application of the MB model to concrete optoelectronic devices, including bulk as well as inter- and intraband quantum well and QD devices. The paper is concluded in Section 10, where dissipation models beyond the Lindblad formalism are discussed.

2. Lindblad Equation

In the following, we consider discrete quantum systems with states $|i\rangle$, where $i = 1 \ldots N$. We restrict ourselves to a single-particle description, valid for carrier densities which are sufficiently low to neglect Pauli blocking, but sufficiently high to neglect electron–hole Coulomb correlation. It has been pointed out that these requirements are often fulfilled in state-of-the-art semiconductor quantum devices which are the main scope of this paper, and that the Lindblad approach introduced below is then well justified. Furthermore, we do not explicitly consider spin dependent effects, even though the Lindblad formalism can be extended accordingly.

The time evolution of an ideal quantum system is famously described by the time dependent Schrödinger equation

$$i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle$$

(1)

with the reduced Planck constant $\hbar$, where the system state vector $|\Psi\rangle$, and generally also the system Hamiltonian $\hat{H}$, depend on time $t$. $|\Psi\rangle$ is a pure state, that is, a coherent superposition of the basis states $|i\rangle$ with $|\Psi(t)\rangle = \sum_i c_i(t)|i\rangle$, where $c_i$ are complex coefficients. In reality, however, no quantum system is perfectly isolated, but rather interacts with its environment. This induces decoherence, that is, loss of quantum coherence in the system, which must be included into any realistic description. The resulting statistical state of the system is generally a mixed state which cannot be represented by the system state vector $|\Psi\rangle$, but rather requires an extended description in terms of the density operator $\rho$. The corresponding density matrix with respect to the chosen
basis states $|i\rangle$ has the elements $\rho_{ij} = \langle i|\rho|j\rangle$, where the diagonal elements $\rho_{ii}$ give the occupation probability of state $|i\rangle$, while the off-diagonal elements $\rho_{ij}$ represent the coherence between $|i\rangle$ and $|j\rangle$. The density operator is positive semidefinite which guarantees that any pure system state $|\Psi\rangle$ has a nonnegative probability, that is, $\langle\Psi|\hat{\rho}|\Psi\rangle \geq 0$. This also implies hermiticity, that is, $\hat{\rho} = \hat{\rho}^\dagger$ and thus $\rho_{ij} = \rho_{ji}^\dagger$, where the dagger and asterisk denote the adjoint and the complex conjugate, respectively. Furthermore, at least for closed systems,[72] the trace must remain constant to ensure particle conservation and is usually normalized to unity, $\text{Tr}(\hat{\rho}) = 1$. The coherent time evolution of the density operator is in the Schrödinger picture described by the von Neumann equation

$$i\hbar\dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$$  \hspace{1cm} (2)

In realistic scenarios, often many degrees of freedom are relevant for the time evolution and must thus be considered. Usually, only part of these degrees of freedom is of direct interest for the application in mind, and solving the full Equation (2) is typically also too demanding. This issue can be addressed by performing a division into a system containing the degrees of freedom which are of primary interest, and a second one with the remaining degrees of freedom which then constitute the environment. In semiconductor quantum devices, the degrees of freedom of interest may be quantized states in a nanostructure such as a quantum well or dot, while decoherence typically arises from interaction with the semiconductor lattice itself, thus acting as the environment. This situation is schematically illustrated in Figure 2. There are various types of interactions, also referred to as scattering mechanisms, which can induce decoherence in the quantum system of interest. These include the interaction with phonons due to (longitudinal- and transverse-optical and -acoustic) thermal lattice vibrations, lattice imperfections in form of impurities (such as dopants), interface roughness or atomic disorder in alloys, as well as piezoelectric fields. Also carrier–carrier interaction can enter the single-particle picture as an additional scattering mechanism.[71,74] For a quantum system interacting with the environment, $\hat{\rho}$ and $\hat{H}$ in Equation (2) refer to the full dynamics of the combined system and environment.

The Hamiltonian $\hat{H}$ can be written as $\hat{H} = \hat{H}_k \otimes \hat{I}_k + \hat{I}_x \otimes \hat{H}_k + \hat{H}_k$, where the Hamiltonians $\hat{H}_k$, $\hat{I}_x$, and $\hat{I}_k$ describe the system $S$, the environment $E$ and the system–environment interaction, $\hat{I}_k$ and $\hat{I}_x$ are the unit operators in the respective Hilbert spaces, and $\otimes$ denotes the tensor product.[75] The reduced density matrix of the system of interest is simply obtained by tracing over the environmental degrees of freedom, $\rho_s = \text{Tr}_E(\hat{\rho})$. This step by itself does obviously not eliminate the dependence of Equation (2) on the environment. Thus, additional assumptions are necessary to arrive at a model for the non-unitary time evolution of $\rho_s$, which is a consequence of eliminating the environmental degrees of freedom. The resulting equation is expected to be similar in structure as Equation (2), that is, a first-order linear differential equation in time for $\rho_s$, where the linearity ensures consistency with the ensemble interpretation of the density matrix.[76] The resulting time-local and Markovian description of the reduced density matrix dynamics is commonly referred to as (quantum) master equation. Its general form can be inferred by posing additional requirements to avoid unphysical behavior. In particular, this includes conservation of unit trace and positive semidefiniteness of the density matrix, as discussed above. Closer inspection reveals that if there exists another system $S'$, an evolution equation for $S$ which ensures positive semidefiniteness of $\rho_s$ can still lead to unphysical time evolution of the combined density matrix for $S$ and $S'$, even if $S'$ does not evolve and is completely decoupled from $S$.[75,76] This problem is cured by demanding complete positivity of the evolution, rather than only the preservation of positive semidefiniteness of $\rho_s$.

From above requirements, the general form of the evolution equation can be inferred by invoking the Kraus theorem,[77] characterizing completely positive trace preserving maps. The resulting master equation is called Lindblad equation.[50,51] Dropping the subscript $S$ from here on for ease of notation, it can be written as

$$\dot{\rho} = -\frac{i\hbar}{\hbar} [\hat{H}, \rho] + \sum_k \left( \hat{L}_k \rho \hat{L}_k^\dagger - \frac{1}{2} \hat{L}_k^\dagger \hat{L}_k \rho - \frac{1}{2} \rho \hat{L}_k^\dagger \hat{L}_k \right) = \mathcal{L}(\rho) + \sum_k \mathcal{D}_k(\rho) = \mathcal{L}(\rho) + \mathcal{D}(\rho) \hspace{1cm} (3)$$

where $\hat{H} = \hat{H}_b + \hat{H}_k$ is the effective Hamiltonian of the reduced system. Here, the Hamiltonian $\hat{H}_b$ describes externally induced perturbations, for example, due to an incident optical field. The description of light–matter interaction requires a time dependent Hamiltonian, which, although lifting the originally assumed time-homogeneity of the Lindblad equation, still gives a valid density matrix evolution.[78,79] In addition, $\hat{H}$ may contain non-dissipative contributions stemming from the interaction with the environment, such as energy shifts.[75] The dissipation is described by the sum term, where the linear operators $\hat{L}_k$ are called Lindblad or (quantum) jump operators, which can in principle be chosen without further restrictions in the Hilbert space of the reduced system. Equation (3) now includes both the coherent dynamics due to the Liouville superoperator $\mathcal{L}(\rho)$, corresponding to Equation (2), and the incoherent dynamics induced by the dissipation superoperator $\mathcal{D}(\rho)$ which contains the interaction with the environment. Besides inferring the Lindblad equation from the requirements given above, Equation (3) can also be microscopically derived, assuming that the quantum system is weakly coupled to a large Markovian environment.[75,80,81]
As mentioned above, we allow for a time dependent Hamiltonian in Equation (3), which is required to include light–matter interaction as envisaged in this paper, and constitutes a slight generalization of the original equation.[80] Occasionally, also time dependent Lindblad operators \( \hat{L}_k(t) \) are used, for example, to model time dependent pumping rates.[82] This also does not affect the physical validity of Equation (3), since conservation of trace and complete positivity are further guaranteed.[78,79] Moreover, Equation (3) with time dependent operators \( \hat{H} \) and \( \hat{L}_k \) is still time-local and also Markovian.[83]

### 2.1. Introduction of Basis States

In principle, the \( N \) basis states of the (reduced) quantum system can be freely selected as long as they span the entire Hilbert space of the \( N \)-level system. In most cases, an orthonormal basis is the preferred option, since it results in more compact expressions and provides a clearer physical interpretation. The choice of energy eigenstates has the distinct advantage that the reduced system Hamiltonian \( \hat{H}_k \) is diagonal. In certain cases, other choices may be preferable, such as a localized (or tight-binding) basis set for the description of tunneling, for example, in double- or multiple-well systems.[84]

Assuming an orthonormal basis so that the unit operator becomes \( \hat{1} = \sum_{\ell=1}^{N} | \ell \rangle \langle \ell | \), Equation (3) can be written as

\[
\partial_t \rho_{ij} = -\frac{i}{\hbar} \sum_\ell \left( \mathcal{H}_\ell \rho_{ij} - \mathcal{H}_j \rho_{i\ell} \right) + \sum_k \sum_p \left[ L_{kp}^\dagger \left( L_k^p \right)^\dagger \rho_{p\ell} - \frac{1}{2} \left( L_k^p \right)^\dagger L_k^p \rho_{i\ell} \right] - \frac{1}{2} \left( L_k^p \right)^\dagger L_k^p \rho_{i\ell} + \sum_{mn} \mathcal{D}_{ijmn} \rho_{mn}
\]

(4)

where \( H_\ell = \langle \ell | \hat{H}_k | \ell \rangle \) and \( L_k^p = \langle \ell | \hat{L}_k | j \rangle \) are the matrix elements of the operators \( \hat{H}_k \) and \( \hat{L}_k \). Also, the superoperators can be represented in form of a matrix, albeit of size \( N^2 \times N^2 \), with elements

\[
\mathcal{L}_{ijmn} = H_m \delta_{jn} - H_j \delta_{im}
\]

(5)

\[
\mathcal{D}_{ijmn} = \sum_k \left[ L_k^m \left( L_k^n \right)^\dagger - \frac{1}{2} \sum_p \left( L_k^p \right)^\dagger L_k^p \delta_{jn} + \left( L_k^m \right)^\dagger L_k^p \delta_{im} \right]
\]

(6)

where \( \delta \) denotes the Kronecker delta. We emphasize that while Equation (6) ensures that there is a matrix representation \( \mathcal{D}_{ijmn} \) for any given set of Lindblad operators, the converse is not necessarily true, and arbitrarily chosen \( \mathcal{D}_{ijmn} \) can produce unphysical results.

### 2.2. Choice of Lindblad Operators

The choice of the \( \hat{L}_k \) for generating a certain time evolution is not unique. In particular, for a given set \( \hat{L}_k \) with \( k = 1, \ldots, K \), the set \( \hat{L}_k' = \sum_k u_{kj} \hat{L}_k \) (also with \( \ell = 1, \ldots, K \)) generates the same dynamics for an arbitrary unitary matrix with dimension \( K \) and elements \( u_{kj} \).[75,85] This can easily be verified by substituting the \( \hat{L}_k \) in Equation (3) with above expression for \( \hat{L}_k' \), and considering that \( \sum_k u_{kj} u_{km}^* = \delta_{jm} \). Furthermore, the \( \hat{L}_k \) might also contain unitary contributions, which can alternatively be included into the Hamiltonian \( \hat{H}_k \). In particular, replacing an operator \( \hat{L}_k \) by \( \hat{L}_k' = \hat{L}_k + \alpha_k \hat{I} \) where \( \alpha_k \) is an arbitrary complex constant with dimension of inverse square root of time, and \( \hat{H}_k \) by \( \hat{H}_k' = \hat{H}_k + (i/2) (\alpha_k \hat{L}_k^* - \alpha_k^* \hat{L}_k) \) generates the same dynamics.[75,85] From the Kraus theorem,[77] it follows that it is always possible to choose the Lindblad operators so that a given non-unitary evolution can be represented by \( K \leq N^2 - 1 \) operators (in addition to \( \hat{H}_k \)) which gives a vanishing contribution in Equation (3)). Formally, such a representation can be constructed by starting from the Kossakowski–Sudarshan form[73] of the Lindblad equation and applying a unitary transformation to convert it to Equation (3).[75]

However, it has been pointed out that the resulting standard form does not give much insight into the underlying physical processes.[83] From a practical point of view, it is more natural to choose the \( \hat{L}_k \) so that they represent certain physical effects. In the following, we will discuss the two most relevant mechanisms, that is, incoherent transitions between states corresponding to hopping transport, and pure dephasing which affects the coherence between two states but does not involve population transfer between them.

#### 2.2.1. Incoherent Transitions

For a transition from a given basis state \( | \alpha \rangle \) to \( | \beta \rangle \) with a rate \( r_{\alpha \rightarrow \beta} \), the associated Lindblad operator is given by

\[
\hat{L}_{\alpha \rightarrow \beta} = r_{\alpha \rightarrow \beta} | \beta \rangle \langle \alpha |
\]

(7)

and Equation (6) for the corresponding superoperator matrix elements yields

\[
\mathcal{D}_{\alpha \beta} = r_{\alpha \rightarrow \beta} \left[ \delta_{\alpha \beta} \delta_{mn} \delta_{\alpha \beta} \delta_{mn} \right] = \frac{r_{\alpha \rightarrow \beta}}{2} \left( \delta_{\alpha \beta} \delta_{mn} \delta_{\alpha \beta} \delta_{mn} \right)
\]

(8)

Inserting Equation (7) into Equation (4), we obtain population changes \( \delta \rho_{\alpha \beta} \delta_{\alpha \beta} \delta_{\alpha \beta} \delta_{\alpha \beta} = r_{\alpha \rightarrow \beta} \rho_{\alpha \beta} \delta_{\alpha \beta} \delta_{\alpha \beta} \delta_{\alpha \beta} \delta_{\alpha \beta} \delta_{\alpha \beta} \) and the superoperator \( r_{\alpha \rightarrow \beta} \) in Equation terms

\[
[r_{\alpha \rightarrow \beta}]_{\alpha \beta} = \sum_{j \neq \alpha} r_{j \rightarrow \alpha} \rho_{\alpha \beta} = r_{\alpha \rightarrow \beta} \rho_{\alpha \beta} \delta_{\alpha \beta}
\]

(9)

where

\[
[r_{\alpha \rightarrow \beta}]_{\alpha \beta} = \sum_{j \neq \alpha} r_{\alpha \rightarrow j}
\]

(10)

is the total outscattering rate from level \( \alpha \). Furthermore, we see that apart from the population changes, \( \hat{L}_{\alpha \rightarrow \beta} \) also contains the
associated lifetime contribution to dephasing, with \([\partial_\beta \rho_{\alpha \beta}]_{\mu \beta} = -(r_{\alpha \beta} / 2) \rho_{\alpha \beta}\) and \([\partial_\beta \rho_{\alpha \beta}]_{\mu \alpha} = -(r_{\alpha \beta} / 2) \rho_{\alpha \beta}\) where \(n \neq \alpha\). This means that population transfer from a state \(|\alpha\rangle\) to \(|\beta\rangle\) induces dephasing not only for this transition, but also for other transitions involving \(|\alpha\rangle\), and ignoring this fact might lead to unphysical results.\(^\text{[72]}\) On the other hand, this implies that the total lifetime contribution to the dephasing rate for a transition \(\alpha \rightarrow \beta\) is with Equation (10) given by \((r_\alpha + r_\beta) / 2\), that is, is obtained from the total outscattering rates for levels \(\alpha\) and \(\beta\). We note that the operator in Equation (7) provides an elementary description of transitions, but does not, for example, take into account correlations between different transition processes.

### 2.2.2. Pure Dephasing

In addition to above discussed population changes, there can be additional mechanisms which do not involve population transfer between the chosen basis states, but cause additional decoherence, resulting in a decay of off-diagonal density matrix elements only.\(^\text{[86–89]}\) This so-called pure dephasing contribution between two levels \(\alpha\) and \(\beta \neq \alpha\) can be described as \([\partial_\beta \rho_{\alpha \beta}]_{\text{pure}} = -\gamma_{\alpha \beta} \rho_{\alpha \beta}\), which also implies \([\partial_\alpha \rho_{\beta \alpha}]_{\text{pure}} = -\gamma_{\alpha \beta} \rho_{\beta \alpha}\) since \(\rho_{\beta \alpha} = \rho_{\alpha \beta}^*\). Here, \(\gamma_{\alpha \beta} \geq 0\) denotes the pure dephasing rate. As can easily be seen, the corresponding dissipation superoperator in Equation (4) can be represented by the matrix elements

\[
\mathcal{D}^{\text{pure}}_{ij, \mu \nu} = -\gamma_{ij} \langle \delta_{\mu \nu} \delta_{ij} \delta_{\mu \nu} \delta_{ij} + \delta_{\mu \nu} \delta_{ji} \delta_{\mu \nu} \delta_{ji} \rangle
\]

The Lindblad operators for pure dephasing must be diagonal in the chosen basis.\(^\text{[85]}\) However, Equation (11) does not generally ensure physical behavior, and thus a representation in terms of Lindblad operators does not always exist.\(^\text{[85]}\) Notably, for \(N \geq 3\), there are constraints on how to select the pure dephasing rates \(\gamma_{ij} \geq 0\) to ensure compatibility with Equation (3), and an ill-considered choice can, for example, easily result in a violation of positive semidefiniteness for \(\rho_{ij} \geq 0\).\(^\text{[85,88]}\) For example, \(\gamma_{12} = \gamma_{23} \geq 2(\gamma_{13}^2 + \gamma_{23}^2 + \gamma_{12}^2 + \gamma_{13}^2 \gamma_{23}^2)^{1/2} \) must hold in three-level systems, which is already violated if only one of the three pure dephasing rates is nonzero.

In two-level systems, pure dephasing is described by a single rate \(\gamma_1 = \gamma_2 = \gamma \geq 0\), and can, for example, be represented by a Lindblad operator \(\hat{L} = (2\gamma)^{1/2}|1\rangle \langle 1|\) or \(\hat{L} = (2\gamma)^{1/2}|2\rangle \langle 2|\), or also by the set \(\hat{L}_1 = (\gamma)^{1/2}|1\rangle \langle 1|\), \(\hat{L}_2 = (\gamma)^{1/2}|2\rangle \langle 2|\). More generally, if the (typically empirical) pure dephasing rate \(\gamma\) is assumed for all transitions of an \(N\)-level system,\(^\text{[90,91]}\) this case can always be represented by Lindblad operators, for example, by the set \(\hat{L}_k = (\gamma)^{1/2}|k\rangle \langle k|\), \(k = 1 \ldots N\).\(^\text{[86]}\)

Taking into account the results of Section 2.2.1, the total phase relaxation due to pure dephasing plus lifetime broadening associated with incoherent transitions is described by the dissipation term

\[
\left[\partial_{\beta} \rho_{\alpha \beta}\right]_{\text{relax}} = -\gamma_{\alpha \beta} \rho_{\alpha \beta} = -\left[(r_\alpha + r_\beta) / 2 + \gamma_{\alpha \beta}\right] \rho_{\alpha \beta}
\]

where \(\gamma_{\alpha \beta} = (r_\alpha + r_\beta) / 2 + \gamma_{\alpha \beta}\) is the total dephasing rate and the \(r_{\alpha,\beta}\) are given by Equation (10).\(^\text{[72]}\)

### 2.2.3. General Case

While physical dissipation channels can often be represented by either incoherent transitions or pure dephasing,\(^\text{[92]}\) see Sections 2.2.1 and 2.2.2, the Lindblad operators should not a priori be restricted to these two forms, but rather be found based on physical considerations.\(^\text{[93,94]}\) Even more, the representation of a dissipative channel as, for example, incoherent transition or pure dephasing, only applies for the chosen basis.\(^\text{[85,90]}\) For illustration, let us assume an \(N\)-level system with orthonormal basis states \(|n\rangle\) and dissipative channels described by a set of Lindblad operators \(\hat{L}_k\). Alternatively, an orthonormal basis with states \(|n'\rangle\) can be used, with \(|n\rangle = \sum_n \langle n'|n\rangle\), which changes the character of the Lindblad operators in the new basis system. As an illustrative example, we restrict ourselves to two relevant levels \((1)\) and \((2)\), which are assumed to be localized in adjacent potential wells, and between which tunneling through the separating barrier occurs. This mechanism plays, for example, an important role in QCLs, which are frequently modeled with a density matrix approach for a discrete quantum system, using localized states to describe the tunneling transport across thick barriers.\(^\text{[62,88,89,95–97]}\) This tunneling process is critically affected by dephasing between the two states involved, which can be modeled by Equation (12).\(^\text{[89,91,95–98]}\) We exemplarily focus on the pure dephasing contribution, which can for a two-level system be described by the Lindblad operator \(\hat{L} = (2\gamma)^{1/2}|1\rangle \langle 1|\) as discussed in Section 2.2.2. Changing to energy eigenstates \(|1'\rangle\) and \(|2'\rangle\) and for simplicity assuming near-degeneracy, we obtain \(|1\rangle = 2^{-1/2}(|1'\rangle + |2'\rangle)\) and \(|2\rangle = 2^{-1/2}(|1'\rangle - |2'\rangle)\).\(^\text{[99]}\) In the energy basis, above Lindblad operator then becomes \(\hat{L} = (\gamma')^{1/2}(|1'\rangle + |1'\rangle + |2'\rangle + |1'\rangle + |2'\rangle)|\) which is not diagonal, that is, does not represent pure dephasing in that basis.

To summarize, the frequently used classification of dissipation channels in incoherent transitions and pure dephasing is not always possible and additionally depends on the chosen basis system, but is frequently used since it allows for an intuitive physical interpretation. Thus, this classification might also be helpful for determining the corresponding dissipative rates based on compact models or by comparison to experimental data.\(^\text{[91,100,101]}\) Consequently, for a given system, a criterion for a convenient choice of basis states might be that the dissipation channels can reasonably well be described in terms of incoherent transitions and pure dephasing, which, for example, motivates the frequent use of localized states to describe tunneling transport through thick barriers.

### 2.3. Conditions for Validity

As discussed in Section 2.2, the dissipation parameters must fulfill certain conditions to ensure physical behavior of the density matrix, which is exactly true if a representation of the dissipation process in terms of Lindblad operators exists. For example, the total dephasing rate of a given transition cannot be smaller than the lifetime broadening contribution due to incoherent transitions, as can be seen from Equation (12). Also, as discussed in Section 2.2.2, the pure dephasing rates cannot be independently chosen for each transition, but must fulfill certain conditions for \(N \geq 3\) levels. Thus, if the experimentally obtained dissipation
rates for a system do not satisfy above conditions, this might indicate that the chosen model is not adequate, for example, that not enough levels are considered.\cite{Note1}

As noted above, the Lindblad equation can also be microscopically derived for a quantum system weakly coupled to a large Markovian environment.\cite{Lindblad1976,Eckern1999,Breuer2002} These assumptions require, in particular, that the coherent system dynamics and relaxation processes occur on a slower timescale than the memory decay of the environment.\cite{Lindblad1976,Eckern1999,Breuer2002} These additional microscopic constraints are not required to ensure completely positive and trace preserving evolution of the density matrix, which is guaranteed by the Lindblad form of Equation (3). However, disregarding the microscopic validity criteria might result in a violation of other laws such as Onsager’s relation.\cite{Onsager1931} On the other hand, it has been pointed out that some of the assumptions usually invoked in microscopic derivations, such as the secular approximation, might be unnecessarily restrictive.\cite{Breuer2002} Eventually, for a description of realistic quantum systems where many degrees of freedom affect the time evolution, there will always be a trade-off between exactness and manageability of the model.\cite{Breuer2002} From a practical point of view, Lindblad-type master equations, such as the MB system, often still yield useful results on the verge of the microscopic validity range, for example, in semiconductor structures interacting with high-intensity fields.\cite{rates2020,macnab2016,macnab2015}

3. Optical Bloch Equations

The most basic quantum system is the two-level system with only \( N = 2 \) relevant states. This can be a natural two-level system with only two eigenstates such as a spin 1/2 particle, or a quasi-two-level system with two strongly coupled states, such as an optical transition in resonance with an electromagnetic field\cite{Rabi1937} or a driven double-well potential.\cite{Walls1995} In an early application of this model, Rabi investigated the interaction of a spin 1/2 particle with a rotating magnetic field by solving the time dependent Schrödinger equation.\cite{Rabi1937} The term “Bloch equations”, in the narrow sense, refers to evolution equations for a dissipative two-level system, first devised to describe the evolution of the nuclear magnetic moment in a magnetic field.\cite{Bloch1940} Here, the interaction with the environment was taken into account by two phenomenological relaxation time constants. This concept was extended to other two-level systems, such as a pair of levels in resonance with a classical optical field.\cite{Bloch1940,DiStefano1940} The resulting evolution equations are occasionally called optical Bloch equations for distinction.\cite{Breuer2002} The optical propagation can be considered by coupling the Bloch model to Maxwell’s equations,\cite{Maxwell1861,DiStefano1940} resulting in the so-called Maxwell–Bloch (MB) equations. In the following, we focus on the interaction of a quantum system with an optical field, where the coupled MB equations have to be used for a combined description of the system dynamics and optical propagation. Here, we will not restrict ourselves to two-level systems, but rather consider the more general case of \( N \geq 2 \) discrete levels. The resulting equations are for \( N \geq 3 \) states occasionally also referred to as a multilevel Bloch/MB model.\cite{Lindblad1976} Furthermore, for the description of dissipative effects due to the system interaction with the environment, the Lindblad formalism introduced in Section 2 will serve as a framework. Sometimes the Lindblad equation, Equation (3), is already referred to as Bloch equations.\cite{Breuer2002} In the following, the (optical) Bloch equations will be regarded as a special form of Equation (3) containing an interaction Hamiltonian \( \hat{H}_i(t) \) to describe light–matter coupling.

3.1. Dipole Approximation

We consider a Hamiltonian of the form \( \hat{H} = (\hat{p} - q\hat{A})^2/(2m) + q\varphi + V \), which models the system’s interaction with a classical optical field, represented by a time and space dependent magnetic vector potential \( \hat{A} = \hat{A}(\hat{r}, t) \) and electric potential \( \varphi = \varphi(\hat{r}, t) \). Here, \( \hat{r} \) and \( \hat{p} \) denote the position and (canonical) momentum operators of the quantum system with the commutator \([\hat{r}, \hat{p}] = i\hbar\delta_{ij} \), which are in position representation given by \( \hat{r} = r \) and \( \hat{p} = -i\hbar\nabla \), and \( V = V(\hat{r}) \) represents the system’s potential energy. Furthermore, \( m \) and \( q \) denote the carrier mass and charge, which are for electrons given by \( m = m_e \) and \( q = -e \), with the elementary charge \( e \). Using the Coulomb gauge \( \nabla A = 0 \), we have \([A, p] = 0 \). Furthermore, assuming a radiation field without free charge contributions gives \( \varphi = 0 \), and \( E = -\partial_t A \) for the corresponding electric field.\cite{Jackson1999} Under these assumptions, we obtain \( \hat{H} = \hat{H}_b + \hat{H}_i \) with the Hamiltonian of the unperturbed system \( \hat{H}_b = \hat{p}^2/(2m) + V \), and the time dependent interaction Hamiltonian\cite{Jackson1999}

\[
\hat{H}_i = -(q/m)\hat{A}\hat{p} + q^2\hat{A}^2/(2m) \tag{13}
\]

The Bloch equations are then obtained from Equation (4) by choosing the energy eigenstates of the system Hamiltonian \( \hat{H}_b \) as basis, resulting in matrix elements \( \hat{H}_{ij} = E_i\delta_{ij} \) where \( E_i \) is the eigenenergy of state \( i \), and

\[
\hat{H}_{ij} = -\frac{q}{m}\langle i|\hat{A}\hat{p}|j\rangle + \frac{q^2}{2m}\langle i|\hat{A}^2|j\rangle \tag{14}
\]

Typically, the field varies on the scale of the optical wavelengths involved, and the system dimensions are much smaller. The carriers then do not experience a spatial field variation across the quantum system, and \( A \) in Equations (13) and (14) can be represented by a space independent vector potential, evaluated at the macroscopic position of the quantum system. In this case, it can be shown by a gauge transformation that the interaction Hamiltonian in Equation (13) is equivalent to

\[
\hat{H}_i = -\hat{d}\mathbf{E}(t) \tag{15}
\]

which corresponds to the interaction Hamiltonian in the widely used (electric) dipole approximation.\cite{Jackson1999,Jackson1999} Here, \( \hat{d} = q\hat{r} \) denotes the system’s dipole operator, and the electric field \( \mathbf{E}(t) \) is taken at the system position. Intuitively, the Hamiltonian in Equation (15) corresponds to the potential energy associated with the force \( q\mathbf{E}(t) \) exerted by the electric field on the carriers.

We note that under some special conditions, such as high harmonic generation\cite{Takayanagi2020} or strong plasmonic confinement in nanophotonic structures,\cite{Ness2019,Langrock2018} the field gradient may become so large that the dipole approximation is not applicable. In this context, we re-emphasize that Equation (15) only assumes a spatially constant field within a given quantum system, but does not neglect the term \( \propto \mathbf{A}^2 \) in Equation (13) and is thus not restricted.
to weak fields, as is sometimes believed. For the interaction Hamiltonian in Equation (15), the mechanical and canonical momentum operators coincide, \( \hat{m} \hat{v} = \hat{p} \). The Hamiltonian of the unperturbed system \( \hat{H}_0 = \hat{p}^2 / (2m) + V \) thus corresponds to the instantaneous energy operator, and a matrix element \( \rho_{ij} \) in the eigenstate basis \( | i \rangle \) of \( \hat{H}_0 \) can be interpreted as the measurable probability of finding the system in the corresponding energy eigenstate.\(^{[110]} \) For the interaction Hamiltonian in Equation (13), the mechanical momentum operator is \( \hat{m} \hat{v} = \hat{p} - q \mathbf{A} \). This complicates the physical interpretation of results, since, for example, the instantaneous energy operator \( \hat{m} \hat{v}^2 / 2 + V \) is different from \( \hat{H}_0 \), which prohibits an interpretation of \( \rho_{ii} \) as a measurable probability.\(^{[110,114,115]} \) These differences also explain why the matrix elements \( H_{ij} \) in Equation (14) for spatially constant \( \mathbf{A} \) and those obtained from Equation (15) deviate from each other.\(^{[110]} \) While both versions of the interaction Hamiltonian lead to identical results for observable quantities as expected, it has been pointed out that the use of approximations, such as the rotating wave approximation discussed in Section 3.5, can cause deviations between the two formulations.\(^{[114,115]} \) In the following, we will use the interaction operator of the form Equation (15).

### 3.2. Optical Bloch Equations in Standard Form

From Equation (4), we obtain with Equation (15) in the dipole approximation the (multilevel) Bloch equations

\[
\partial_t \rho_{ij} = -i \omega_{ij} \rho_{ij} + \frac{i}{\hbar} \sum_{\ell} (\hat{d}_i \rho_{\ell j} - \hat{d}_j \rho_{i \ell}) E + \sum_{\ell \mu} D_{ij\ell\mu} \rho_{\mu \ell} \tag{16}
\]

with the transition frequencies \( \omega_{ij} = (E_i - E_j) / \hbar \). If we furthermore restrict the description of dissipative effects to incoherent transitions and dephasing, Equations (9) and (12), Equation (16) simplifies to

\[
\partial_t \rho_{ij} = -i \omega_{ij} \rho_{ij} + \frac{i}{\hbar} \sum_{\ell} (\hat{d}_i \rho_{\ell j} - \hat{d}_j \rho_{i \ell}) E - \gamma_{ij} \rho_{ij}, \quad i \neq j \tag{17a}
\]

\[
\partial_t \rho_{ii} = \frac{i}{\hbar} \sum_{\ell} (\hat{d}_i \rho_{\ell i} - \hat{d}_i \rho_{i \ell}) E + \sum_{j \neq i} r_{j \rightarrow i} \rho_{j j} - r_i \rho_{ii} \tag{17b}
\]

Although quantum optoelectronic devices can in principle comprise a single isolated quantum system, for example, a QD,\(^{[116,117]} \) in general they are based on extended nanostructures such as quantum well structures, or an ensemble of many quantum systems such as multi-quantum-dot structures. This requires a position resolved model, where the device is described by a representative quantum system with density matrix \( \rho_i (x, t) \) at each device position \( x \). Furthermore, also the parameters \( \omega_{ij}, \hat{d}_{ij}, \gamma_{ij}, r_{j \rightarrow i}, \) and \( r_i \) in Equations (16) and (17) generally depend on \( x \) for inhomogeneous device structures,\(^{[118,119]} \) such as multi-section lasers.\(^{[120–122]} \)

![Figure 3. Band structure of gallium arsenide (GaAs), obtained based on a simple pseudo-potential tight-binding method without spin-orbit coupling.\(^{[123]} \) Shown is the valence band (dashed lines), the conduction band (solid line), and the parabolic dispersion relation assumed for the Γ valley in effective mass approximation (dotted line).](image)

### 3.3. Optical Dipole Matrix Element

The Hamiltonian part of the Bloch equations, Equations (16) and (17), requires the dipole matrix element vectors \( \hat{d}_i \) of the optical transitions and the eigenenergies of the quantized states as an input. These can be computed from models derived from the stationary Schrödinger equation, such as the effective mass or \( \mathbf{k} \cdot \mathbf{p} \) approach, as shortly discussed in the following.

In Figure 3, the band structure of GaAs as an exemplary direct bandgap semiconductor material is displayed. Shown is the conduction band (solid line) and the valence band (dashed lines), consisting of heavy hole, light hole, and split-off band. The holes tend to accumulate near the valence band maximum which is always at the Γ point where the crystal wavevector is \( \mathbf{k} = 0 \). For direct bandgap semiconductors, the global conduction band minimum where the electrons accumulate happens to be also at the Γ point, and thus conservation of crystal momentum can be satisfied for radiative electron–hole recombination. This process is much less likely in indirect bandgap semiconductors, where the global conduction band minimum is not at the Γ point and the process must additionally involve a phonon or crystal defect to achieve momentum conservation.

Assuming a direct bandgap semiconductor, it is practical to write the full wavefunction \( F_i (\mathbf{r}) \) of the initial and final state as a product of periodic Bloch function \( u_{\mathbf{k}} (\mathbf{r}) \) at the Γ point of band \( v_i \) and an envelope wavefunction \( \varphi_i (\mathbf{r}) \) describing the slowly varying spatial modulation of the full wavefunction across the nanostructure.\(^{[124]} \) While a quantized state in a given band generally also contains contributions from neighboring bands, in a first approximation, only the contribution of the dominant band is considered.\(^{[124]} \)

\[
F_i (\mathbf{r}) = u_{\mathbf{k}_i} (\mathbf{r}) \varphi_i (\mathbf{r}) \tag{18}
\]

In quantum well structures, the material composition changes only along the growth direction \( x \). Here, quantum confinement
only occurs in \( x \) direction, while the carriers can move freely in the \( yz \)-plane. Thus, we can make the ansatz

\[
\psi_i(r) = S^{-1/2} \psi_i(x) \exp(ik_y y + ik_z z)
\]

Here, \( S \) is the in-plane cross section area, \( k = [k_y, k_z]^T \) denotes the in-plane wavevector in the \( yz \)-plane where \( T \) indicates the transpose, and \( \psi_i(x) \) is the (generally \( k \) dependent) 1D envelope wavefunction in confinement direction. In Figure 4, the full wavefunctions \( F_i \) and corresponding envelope wavefunctions \( \psi_i \) are schematically illustrated for the two lowest conduction band states and the valence band ground state of a quantum well. Similar considerations apply to quantum wires, where quantum confinement occurs in two dimensions while the carriers can move freely along the third coordinate. In QDs, the carriers are confined in all three dimensions.

### 3.3.1. Computation of Envelope Wavefunction

Neglecting the coupling between conduction and valence bands, the simplest model for computing \( \psi_i(r) \) in a quantum structure is the Ben Daniel–Duke model, which works well for low-lying conduction band states in the \( \Gamma \) valley and generally at the heavy hole valence band maximum.\(^{[124]}\) Here, we describe the dispersion relation between energy and wavevector around the \( \Gamma \) point by \( E(k) = V + h^2 k^2 / (2m^*) \) which corresponds to a second-order expansion, as illustrated by the dotted line in Figure 3. The position dependent material composition in nanostructures causes the effective mass \( m^* \) and band edge energy \( V \) to depend on \( r \), where \( V \) additionally contains the externally applied bias. Within this model, the stationary effective mass Schrödinger equation is given by\(^{[124]}\)

\[
0 = -\frac{h^2}{2m^*(r)} \nabla^2 \psi_i(x) + V(r) - E_i \psi_i(x)
\]

where \( E_i \) denotes the eigenenergy of state \( i \). For the valence band, commonly the hole picture is adopted to avoid a negative effective mass in Equation (20). For the transition between a conduction band electron state with eigenenergy \( E_i \) and a valence band hole state with energy \( E_j \), the transition energy is then given by \( E_i + E_j + E_g \) where \( E_g \) denotes the bandgap energy, that is, the energy difference between valence band maximum and conduction band minimum. In quantum well systems, \( m^* \) and \( V \) depend on the \( x \) coordinate, and Equation (20) can be reduced to the 1D effective mass equation by inserting Equation (19). Similar considerations apply to quantum wires where \( m^* \) and \( V \) only depend on two coordinates.

The Ben Daniel–Duke model in Equation (20) can be extended, for example, by accounting for band bending due to space charge effects in the potential, which is self-consistently included by solving Equation (20) together with the Poisson equation.\(^{[125,126]}\) Furthermore, an energy dependent effective mass can be introduced to include nonparabolicity effects associated with the deviation of the dispersion relation from the parabolic form assumed above.\(^{[127,128]}\)

A further refined treatment of the conduction and valence bands, which accounts for band coupling, is usually performed based on \( k.p \) theory, initially proposed by Kane\(^{[129,130]}\) and Luther and Kohn.\(^{[131]}\) Here, the envelope wavefunctions are not scalar, but a multicomponent vector containing contributions from all the bands considered. In many structures, strain arising from the lattice mismatch between the different semiconductor compounds plays an important role, and can be considered based on the Bir–Pikus model.\(^{[132]}\) For modeling interband devices, eight-band \( k.p \) is a common option which considers the top three valence bands and the lowest conduction band, along with spin orientation.\(^{[124,133]}\) This approach is routinely applied to nanostructures, such as quantum dots,\(^{[134]}\) wires,\(^{[135]}\) and wells.\(^{[136]}\) If only valence band states are considered, a restriction to six bands is possible.\(^{[137]}\) This approach is sometimes also combined with Equation (20) for the conduction band, assuming that it is decoupled from the valence bands. On the other hand, it has been found that for certain cases, eight-band \( k.p \) is not accurate enough. For example, a 14-band \( k.p \) approach which also includes the second conduction band in III-V semiconductors has been developed to obtain a more accurate conduction band dispersion relation at higher energies,\(^{[138]}\) and 14-band \( k.p \) has also yielded improved results for SiGe/Si heterostructures.\(^{[139]}\)

### 3.3.2. Inter- and Intraband Dipole Matrix Elements

The dipole matrix element is best evaluated by computing the expectation value of the momentum operator \( \mathbf{p} = -ih \mathbf{\nabla} \). Employing the product rule and exploiting the fact that the periodic Bloch functions and envelope wavefunctions vary on two different length scales, we can with Equation (18) write\(^{[140]}\)

\[
\langle F_i | \mathbf{p} | F_j \rangle \approx \langle \psi_i | \mathbf{p} | \psi_j \rangle = \langle u_i | \mathbf{p} | u_j \rangle + \langle u_i | u_j | \psi_i | \mathbf{p} | \psi_j \rangle
\]

For transitions between conduction and valence band states, the first term dominates because the Bloch functions vary much more rapidly than the envelope wavefunctions. Using \( \langle F_i | \mathbf{p} | F_j \rangle = im_e E_g \langle F_i | \mathbf{k} | F_j \rangle / \hbar \) with the electron mass \( m_e \) and
bandgap energy $E_g^{[141]}$, the interband dipole matrix element can then in a first approximation be written as

$$\langle F_i | \hat{F} | F_j \rangle = -i\hbar m_e^{-1} E_g^{-1} (u_{ni} | \hat{p} | u_{nj}) \langle \psi_i | \psi_j \rangle$$ \hspace{1cm} (22)

For intraband optical transitions, we have $n_i = n_j$, $(u_{ni} | \hat{p} | u_{nj}) = 0$ and $(u_{ni} | u_{nj}) = 1$, and thus Equation (21) yields $\langle F_i | \hat{p} | F_j \rangle \approx \langle \psi_i | \psi_j \rangle$ and analogously

$$\langle F_i | \hat{d} | F_j \rangle \approx \langle \psi_i | \hat{d} | \psi_j \rangle$$ \hspace{1cm} (23)

In quantum well systems, confinement only occurs in the growth direction $x$, and the envelope wavefunction has the form given by Equation (19). For transitions between a conduction band state $|\psi_i, k\rangle$ and a valence band state $|\psi_j, k\rangle$, $\langle \psi_i | \psi_j \rangle = \langle \psi_i | \psi_j \rangle \delta_{k,k'}$, that is, the optical transition is $k$ conserving. The absolute value of the dipole matrix element can be approximately written as

$$|e| F_i | \hat{F} | F_j | k' \rangle | = c_{ij} E_g^{-1} P_o \langle \psi_i | \psi_j \rangle \delta_{k,k'}$$ \hspace{1cm} (24)

where $e$ denotes the polarization direction of the electric field, and $P_o \approx 0.85 \ldots 1\, \text{nm} \times \text{eV}$ for most common semiconductors.\textsuperscript{[140]} For transitions between conduction band and heavy hole states, $c_{ij} = 2^{-1/2}$ for polarization in in-plane direction and $c_{ij} = 0$ for polarization in growth direction. For transitions between conduction band and light hole states, $c_{ij} = 6^{-1/2}$ for polarization in in-plane direction and $c_{ij} = 2 \times 6^{-1/2}$ for polarization in growth direction. For interband transitions occurring between quantized levels in the conduction band of quantum wells, as are, for example, employed for QCLs, the envelope wavefunctions again assume the form Equation (19). The dipole matrix element between an initial state $|\psi_i, k\rangle$ and a final state $|\psi_j, k\rangle$ is then with Equation (23) given by $d_{ij,k,k'} = d_{ij} \delta_{k,k'}$, where

$$d_{ij} = \langle \psi_i | \hat{d} | \psi_j \rangle = -ee \int \psi_i^* \hat{d} \psi_j \, dx$$ \hspace{1cm} (25)

Here, $e\,\mathbf{e}$ denotes the unit vector in $x$ direction, and only the dipole matrix element for polarization in growth direction $x$ is nonzero. Notably, this is different from transitions between conduction band and heavy hole states in quantum wells where the $x$ component of $d_{ij}$ is zero, as discussed above. In Figure 5, the possible field polarization directions for interband (Figure 5a,b) and intraband (Figure 5c) transitions are indicated. For quantum well lasers, Figure 5a–c correspond to the standard edge-emitting, vertical-cavity surface-emitting, and quantum cascade laser.

In quantum dots, the uppermost valence band eigenstates usually exhibit heavy hole character.\textsuperscript{[142–145]} Thus, band coupling effects can often be neglected in Equation (22) for interband transitions between the heavy-hole-like states and low-lying conduction band states. Within the framework of these assumptions, only optical dipole transitions between hole and electron states with equal quantum numbers are allowed, and the envelope wavefunction overlap in Equation (22) typically approaches $\langle \psi_i | \psi_j \rangle \approx 1$ for the allowed transitions.\textsuperscript{[146,147]} The symmetry of the wavefunctions can however be affected by inhomogeneities in shape and composition of the quantum dots as well as piezoelectric fields, resulting in additional weakly allowed transitions.\textsuperscript{[148,149]} Moreover, due to the strong confinement in quantum dots, Coulomb interactions tend to play a pronounced role, causing energy shifts as well as somewhat altered selection rules. Such effects can be included in a more complete description based on the electron–hole-pair picture, which replaces the single-carrier envelope wavefunctions $\psi_i$ and $\psi_j$ in Equation (22) by expressions for the excited electron–hole pair state and the corresponding ground state.\textsuperscript{[146,148]} Intraband transitions, which are mainly relevant in the context of quantum dot infrared photodetectors, are again described by Equation (23).

### 3.4. Nonredundant Density Matrix Representation

For a discrete-level system with $N$ eigenstates $|j\rangle$, the density matrix contains $N^2$ real diagonal elements and $N^2 - N$ complex off-diagonal elements which are related by $\rho_{ij} = \rho_{ji}^*$. Furthermore, considering the trace condition $\text{Tr}(\hat{\rho}) = 1$, the density matrix can be represented by $N^2 - 1$ nonredundant, real-valued elements, which are conveniently written as a vector $\mathbf{S}$. This nonredundant representation is, for example, achieved by the coherence vector (or pseudospin) representation;\textsuperscript{[150]} which has also been found useful for numerically efficient implementations of the MB equations.\textsuperscript{[53,131–133]} For this purpose, the density matrix operator $\hat{\rho}$ is composed as

$$\hat{\rho} = \frac{1}{N} \mathbf{j} + \frac{1}{2} \sum_{j=1}^{N^2-1} S_j \delta_j$$ \hspace{1cm} (26)

Here, $\delta_j$ are generators of the Lie algebra of SU$(N)$ which are traceless Hermitian operators fulfilling the condition...
\(\text{Tr}(\hat{s}_i \hat{s}_k) = 2\delta_{jk},\) and \(\hat{I}\) is the identity operator. \(\hat{I}\) and \(\hat{s}_j\) can be represented by corresponding \(N \times N\) matrices. A possible choice for the generators \(\hat{s} = \{\hat{a}_1, \hat{a}_1^\dagger, \ldots, \hat{a}_n, \hat{a}_n^\dagger, \ldots, \hat{w}_{N-1}\}\) consists of \(N(N - 1)/2\) generator pairs

\[
\hat{a}_{jk} = \hat{t}_{jk} + \hat{t}_{kj} \\
\hat{v}_{jk} = -i(\hat{t}_{jk} - \hat{t}_{kj})
\]  

and \(N - 1\) generators

\[
\hat{w}_l = -[2l^{-1}(l + 1)]^{1/2} \sum_{j=1}^{l-1} \left(\hat{t}_{jt} - \hat{t}_{jt+1,j+1}\right)
\]

where \(\hat{t}_{jk} = |j\rangle\langle k|\) is the transition-projection operator, and the indices satisfy \(1 \leq j < k \leq N\) and \(1 \leq l \leq N - 1\). For \(N = 2\) and \(N = 3\), these generators produce the Pauli and the Gell-Mann matrices, respectively.

The elements of the coherence vector \(\mathbf{S}\) are defined as \(S_j = \text{Tr}(\hat{\rho} \hat{s}_j)\) using the Hilbert–Schmidt inner product. Since both \(\hat{\rho}\) and the generators \(\hat{s}_j\) are Hermitian, the vector elements are real. A similar transform can be applied to the Lindblad equation. Inserting Equation (26) into Equation (3) and applying \(\text{Tr}\{\hat{s}_i\}\) yields

\[
\text{Tr}\{\partial_t \hat{s}_i\} = \frac{1}{2} \sum_{j=1}^{N^2-1} \partial_t S_j \delta_{ji} \delta_{sk} \\
= \frac{1}{2} \sum_{j=1}^{N^2-1} \partial_t S_j \text{Tr}\{\hat{s}_j \hat{s}_k\} \\
= \partial_t S_k
\]

for the left hand side. For the right hand side, we can write

\[
\text{Tr}\{\mathcal{L}\hat{s}_i\} + \mathcal{D}(\hat{\rho})\hat{s}_i) = \text{Tr}\{\mathcal{L}(\hat{\rho})\hat{s}_i\} + \text{Tr}\{\mathcal{D}(\hat{\rho})\hat{s}_i\}
\]

\[
= \frac{1}{2} \sum_{j=1}^{N^2-1} \text{Tr}\{\mathcal{L}(\hat{\rho})\hat{s}_j\} S_j \\
= \frac{1}{2} \sum_{j=1}^{N^2-1} \text{Tr}\{\mathcal{D}(\hat{\rho})\hat{s}_j\} S_j
\]

since both superoperators \(\mathcal{L}\) and \(\mathcal{D}\) are linear. Noting that \(\mathcal{L}(\hat{I}) = 0\) and arranging Equations (29) and (30a)–(30c) in matrix-vector form yields

\[
\partial_t \mathbf{S} = (\mathbf{L} + \mathbf{D})\mathbf{S} + \mathbf{S}^{\mathcal{N}}
\]

where \(\mathbf{L}\) and \(\mathbf{D}\) are \((N^2 - 1) \times (N^2 - 1)\) real matrices and \(\mathbf{S}^{\mathcal{N}}\) denotes the equilibrium coherence vector.

Alternatively, one can start from Equation (4), where the superoperators \(\mathcal{L}\) and \(\mathcal{D}\) are represented as \(N^2 \times N^2\) matrices. This Liouville space representation was used, for example, in ref. [154], where column-major order was applied to map the indices \((i, j) \mapsto k\) and \((m, n) \mapsto l\). In this case, the density matrix is represented as \(N^2\) column vector \(\mathbf{R}\), and the Lindblad equation reads\[^{154}\]

\[
\partial_t \mathbf{R} = \left(-\frac{i}{\hbar} \mathcal{L} + \mathcal{D}\right) \mathbf{R}
\]

where \(\mathcal{L} = \hat{H}^\dagger \otimes \hat{I} - \hat{I} \otimes \hat{H}\) and

\[
\mathcal{D} = \sum_k \left[\hat{E}_k^{\dagger} \otimes \hat{L}_k - \frac{1}{2} \left(\hat{E}_k^{\dagger} \hat{L}_k \otimes \hat{1} + \hat{1} \otimes \hat{L}_k \hat{E}_k\right)\right]
\]

Here, \(\otimes\) denotes the Kronecker product. Then, since the Hilbert–Schmidt inner product reads \(\text{Tr}(\hat{a} \hat{b}) = a^\dagger b = b^\dagger a\) in this representation, where the vectors \(a\) and \(b\) are the matrices \(\hat{a}\) and \(\hat{b}\) in column-major order, we can write the transform from Liouville space to the coherence vector representation as

\[
\mathbf{S}_j = \text{Tr}\{\hat{\rho} \hat{s}_j\} = \mathbf{s}_j^\dagger \mathbf{R} \quad \mathbf{S} = \mathbf{T}^\dagger \mathbf{R}
\]

where the columns of the transformation matrix \(T\) are the generators \(\hat{s}_j\) in column-major order. Conversely, the vector \(\mathbf{R}\) can be recovered by

\[
\mathbf{R} = \frac{1}{N} \mathbf{I} + \frac{1}{2} \mathbf{T} \mathbf{S}
\]

for the left hand side. For the right hand side, we can write

\[
\partial_t \mathbf{S} = \frac{1}{2} T^\dagger \mathbf{S} \left(-\frac{i}{\hbar} \mathcal{L} + \mathcal{D}\right) \frac{1}{2} \mathbf{T} \mathbf{S} + \frac{1}{N} \mathbf{T}^\dagger \mathbf{D} \mathbf{I}
\]

and simplify the result by left-multiplication with \(T^\dagger\) to

\[
\partial_t \mathbf{S} = \left(-\frac{i}{2\hbar} \mathcal{L}^\dagger \mathcal{L} T + \frac{1}{2} T^\dagger \mathcal{D} \mathcal{L} T\right) \mathbf{S} + \frac{1}{N} \mathcal{L}^\dagger \mathcal{L} \mathbf{I}
\]

where we used the orthogonality of the generators \((\frac{i}{2} \mathcal{L}^\dagger \mathcal{L} = I, \) where \(I\) is the \(N^2 \times N^2\) identity matrix) and the fact that the commutator of the identity is zero \((\mathcal{L} \mathcal{I} = 0)\). This corresponds to Equation (31).

As we shall see in Section 4, the derivative of the macroscopic polarization \(\partial_t \mathbf{P}_\mathcal{N}\) has to be calculated for the Maxwell–Bloch equations. Naturally, it must be expressed as function of the vector \(\mathbf{S}\). By replacing the trace operation and inserting the transformation rule, we can write for this term

\[
\partial_t \mathbf{P}_\mathcal{N} = n_{\mathcal{N}} \text{Tr}\{\partial_t \hat{\rho} \hat{d}\} = n_{\mathcal{N}} \mathbf{u}^\dagger \mathbf{R} = \frac{1}{2} n_{\mathcal{N}} \mathbf{u}^\dagger T[(\mathbf{L} + \mathbf{D})\mathbf{S} + \mathbf{S}^{\mathcal{N}}]
\]

where \(\mathbf{u}\) is the vectorized dipole moment operator and \(n_{\mathcal{N}}\) denotes the carrier number density. Note that the elements of \(\mathbf{u}\) could be vectors themselves, depending on whether one or more dimensions are considered.

Using the dipole approximation, Equation (15), we plug in the Hamiltonian \(\hat{H} = \hat{H}_B - \mathbf{dE}(t)\), which can be represented with two matrices \(\mathcal{L}_0\) and \(\mathcal{L}_1\) in Liouville space (and two matrices \(L_0\)
and $L_1$ in coherence vector representation, respectively). Since
\[ u | L_1 \rangle = -u \left[ \hat{d} \hat{E}(t) \otimes I - I \otimes \hat{d} \hat{E}(t) \right] \]
\[ = -\left[ \text{vec} \left( \hat{d} \hat{E}(t) \right) \otimes I u - I \otimes \text{vec} \left( \hat{d} \hat{E}(t) \right) u \right] \]
\[ = -\left[ \text{vec} \left( \hat{d} \hat{d} \hat{E}(t) \right) - \text{vec} \left( \hat{d} \hat{E}(t) \hat{d} \right) \right] = 0 \] (39)
where vec denotes the vectorization of an operator, vec($\hat{d}$) = $u$, and the Hermitian property of the operators involved as well as the properties of the Kronecker product have been exploited, the polarization does not depend on the electric field and Equation (38) can be refined as
\[ \partial_t \rho_i = \frac{1}{2} \text{tr} [ (L_0 + D) S + S^\dagger ] \] (40)

3.5. Rotating Wave Approximation

The Bloch equations (17) are solvable only under special conditions, like $|\Delta M| = 1$ transitions in hydrogen-like atoms excited with circularly polarized light.\cite{14,49} In particular, closed analytical solutions do not exist for the basic and very important case of excitation with a monochromatic, linearly polarized field.\cite{45} Furthermore, the numerical solution of the Maxwell–Bloch equations requires high spatiotemporal resolution since the fields as well as the off-diagonal density matrix elements in Equation (17) oscillate with the optical period. For these reasons, the rotating wave approximation (RWA) is commonly invoked, which significantly reduces the numerical burden and enables an analytical treatment of the Bloch equations, at least for incident monochromatic radiation and some other relevant cases.

The RWA is only applicable for not too broadband optical fields, which can then be separated into a slowly varying amplitude, given in complex notation by $E(x, t) = |E(x, t)| \exp[i\phi(x, t)]$, and a rapidly oscillating carrier with frequency $\omega_c > 0$. We note that there is no unique definition of $\omega_c$, but rather any choice which ensures that all relevant spectral components are close to $\omega_c$ will suffice (for optical fields with symmetric power spectra, it obviously makes sense to pick the center frequency). In complex notation, the electric field can then be written as
\[ E = \frac{1}{2} \tilde{E} \exp(-i\omega_c t) + \text{c.c.} \] (41)
where c.c. denotes the complex conjugate. Furthermore, assuming that all transitions between pairs of states $i$ and $j$ with non-negligible coupling to the optical field are in near-resonance, $|\omega_{ij}| \approx \omega_c$, the corresponding off-diagonal density matrix elements are transformed into a rotating reference frame,
\[ \rho_{ij} = \eta_{ij} \exp \left[ -i \text{sgn}(\omega_{ij}) \omega_c t \right] \] (42)
where sgn denotes the sign function. Inserting Equations (41) and (42) in Equation (17), multiplying both sides of Equation (17a) with $\exp[i\text{sgn}(\omega_{ij}) \omega_c t]$ and applying the RWA, that is, discarding all rapidly oscillating terms $\propto \exp(\pm i \omega_c t)$ and $\exp(\pm 2i \omega_c t)$,\cite{49} we obtain
\[ \partial_t \eta_{ij} = i \Delta_{ij} \eta_{ij} + i \left( \frac{1}{2\hbar} (\rho_{ij} - \rho_{ji}) d_{ij} \right) \left\{ \frac{E}{E^2} \right\} - \gamma_{ij} \eta_{ij}, \omega_{ij} \{ > 0 \} < 0 \} \] (43a)
\[ \partial_t \rho_{ii} = \frac{1}{\hbar} \sum_{\omega_{ij} > 0} \gamma \{ d_{ij} \eta_{ij} E^2 \} + \frac{1}{\hbar} \sum_{\omega_{ij} < 0} \gamma \{ d_{ij} \eta_{ij} E \} \]
\[ + \sum_{j \neq i} r_{ij} \rho_{ij} - r_{ii} \rho_{ii} \] (43b)
with $\Delta_{ij} = \text{sgn}(\omega_{ij})(|\omega_c| - |\omega_{ij}|)$. As discussed above, the RWA is only applicable if the near-resonance condition is fulfilled, that is, all significant spectral components $E(\omega)$ of the field are close to resonance with all relevant optical transitions at frequencies $\omega_{ij}$, $|\omega - |\omega_{ij}|| < |\omega_{ij}|$. As a second condition, the interaction energy must be so small that the eigenfrequencies of the quantum system are not considerably perturbed,\cite{49} that is, $|d_{ij} E|/\hbar \ll |\omega_{ij}|$.

4. Maxwell–Bloch Equations

The optical field propagation in the device is classically described in terms of Maxwell’s equations. Assuming that the magnetization is negligible at optical frequencies, we can write Faraday’s and Ampère’s law for the electric field $E$ and magnetic field $H$ as
\[ \nabla \times E = -\mu_0 \partial_t H \] (44a)
\[ \nabla \times H = \varepsilon_0 \varepsilon_r \partial_t E + \sigma E + J_q \]
\[ = \varepsilon_0 \varepsilon_r \partial_t E + \sigma E + J_q + \partial_t P_q \] (44b)
where $E$, $H$, and $J_q$ are functions of both $t$ and $x$. $J_q = J_\parallel + \partial_t P_q$ denotes the total current density contribution of the quantum systems. Here, $J_\parallel$ and $\partial_t P_q$ correspond to the current density due to free carrier motion and the polarization current density, respectively, where $P_q$ is the macroscopic polarization. In Figure 6, the coupled modeling of the field propagation and the quantum system dynamics is schematically illustrated. For extended nanostructures such as quantum well structures or ensembles of QDs, the medium must be described by a representative quantum system at each position $x$. The Bloch equations, Equation (17), are coupled to Equation (44) via $E$. On the other hand, Equation (44) is coupled to Equation (17) via $J_\parallel$. For practical reasons, we consider the background polarization due to the host medium separately by the (generally $x$ dependent) dielectric constant $\varepsilon(x)$, where we have for now neglected any frequency dependence, and assumed linearity and isotropy of the host. Likewise, we include the absorption of the host medium by a scalar conductivity $\sigma(x)$, which gives rise to an ohmic current contribution $\sigma E$ in Equation (44b). Furthermore, $\varepsilon_0$ and $\mu_0$ denote the vacuum permittivity and permeability, respectively.
4.1. Macroscopic Polarization and Current Density

Here, as above, we use the position variable \( \mathbf{r} \) to resolve microscopic behavior, while the variable \( \mathbf{x} \) describes the position in the modeled device or geometry and refers to macroscopic dependencies, obtained from microscopic models by adequate ensemble averaging. In Maxwell’s equations, the total macroscopic current density contribution of the quantum systems is given by \( \mathbf{J}_f(x, t) = \mathbf{J}_i(x, t) + \partial_t \mathbf{P}_q(x, t) \), where the free charge current density \( \mathbf{J}_f \) and polarization current density \( \partial_t \mathbf{P}_q \) contain the contributions due to free and bound charges, respectively. In optoelectronic devices, \( \mathbf{J}_i \) is, for example, induced by electrical pumping or generated by the photovoltaic effect, while \( \partial_t \mathbf{P}_q \) is associated with the bound charge oscillations induced by the optical field. Microscopically, in nanostructured devices the carriers in bound or quasi-bound states may contribute to \( \partial_t \mathbf{P}_q \) by coherent or incoherent interaction with the optical field, as well as to \( \mathbf{J}_i \) via coherent transport such as tunneling and incoherent transport such as scattering-induced hopping. Thus, it makes sense to treat polarization and current density together.

The macroscopic polarization \( \mathbf{P}_q \) can be obtained from the dipole moment of a quantum system, given by the expectation value of the dipole moment operator \( \langle \mathbf{d}(t) \rangle = \text{Tr}[\hat{\mathbf{d}}(t)\hat{\rho}] \). \( \mathbf{P}_q \) at a position \( x \) is then obtained by summing over the quantum systems in a volume \( V_p \) around \( x \),

\[
P_q = V_p^{-1} \sum_i \langle \hat{d}_i \rangle
\]

where \( V_p \) is chosen big enough to obtain a smooth dependence of \( \mathbf{P}_q \), but small enough so that spatial variations on classical length scales can still be resolved. For a large ensemble of identical systems with carrier number density \( n_{1D} \), the polarization is then given by

\[
P_q = n_{1D} \langle \hat{d} \rangle = n_{1D} q \text{Tr}[\hat{r}\hat{\rho}]
\]

where \( \hat{\rho} \) is the density operator of a representative quantum system at position \( x \). On the other hand, the electric current in the quantum system can be computed from the expectation value of carrier velocity \( \langle \hat{\mathbf{v}} \rangle \) in the system, where the velocity operator is defined in the Heisenberg picture by the time derivative of the position operator \( \hat{\mathbf{r}}_i, \hat{\mathbf{v}}_i = \partial_t \hat{\mathbf{r}}_i \). For the coherent contribution corresponding to the Hamiltonian part in Equation (3), we then obtain with the Ehrenfest equation \( \langle \hat{\mathbf{v}} \rangle = \langle \partial_t \hat{\mathbf{r}} \rangle \), where we have dropped the index \( H \) since expectation values for physical observables are independent of the chosen picture. In the Schrödinger picture, we thus obtain \( \langle \hat{\mathbf{v}} \rangle = \langle \partial_t \hat{\mathbf{r}} \rangle = \partial_t \text{Tr}[\hat{\mathbf{r}}\hat{\rho}] \), which is also valid for the incoherent contribution induced by the Lindblad operator term in Equation (3). Thus, \( I = q \langle \hat{\mathbf{v}} \rangle / L \) corresponds to the current through an individual (single-carrier) quantum system, where \( L \) indicates the system length in the direction of current flow, and \( L / \langle \hat{\mathbf{v}} \rangle \) is the transit time of the carrier through the system. Again, averaging over a large ensemble of identical systems, we obtain the macroscopic current density \( \mathbf{J}_f = n_{1D} q \text{Tr}[\hat{\mathbf{r}}\hat{\rho}] \). We note that this result is the same as for the polarization current density, obtained by taking the time derivative of Equation (46), which reflects the fact that the carriers of the quantum system are responsible for both the free charge current and polarization current. Even more, from a microscopic standpoint, this distinction is inappropriate for our case. Thus we can write

\[
\mathbf{J}_q = n_{1D} q \text{Tr}[\hat{r}\hat{\rho}]
\]

where \( \hat{\rho} \) again describes a representative quantum system at position \( x \), and \( \hat{\rho} \) given by Equation (3), contains both the coherent and incoherent dynamics. Assuming an \( N \)-level system with orthonormal basis states \( |j\rangle \), Equation (47) can with the dipole matrix element \( d_{ij} = q \langle (i|\mathbf{r}|j) \rangle \) be written as

\[
\mathbf{J}_q = n_{1D} \sum_{i,j} d_{ij} \partial_t \rho_{ij}
\]

with \( \partial_t \rho_{ij} \) given by Equation (4) or (17).

A widely used criterion to distinguish between the macroscopic free charge and polarization current contributions in Equation (48) is the frequency range, where commonly \( \partial_t \mathbf{P}_q \) is expected to contain frequencies in the range of the driving optical field spectrum, while \( \mathbf{J}_f \) covers the low-frequency and direct current contributions. In this context, we point out that due to nonlinear optical mixing, the polarization generally contains up- and down-converted components. This especially applies to nanostructured optoelectronic devices where giant optical non-linearities can be artificially engineered, and are actively exploited in both the optical and terahertz regime.  

On the other hand, the electric current can contain components up to tens of GHz due to external modulation or back-coupling of the optical dynamics to the electrical circuitry. Notably, in QCLs embedded into a micro-strip line, strong coupling of the co-propagating microwave current modulation and optical waveform has recently been found, indicating that a clear differentiation between free and polarization current contributions is not always possible. However, as pointed out above, such a distinction is also not necessary since the current density and polarization appear as \( \mathbf{J}_q = \mathbf{J}_f + \partial_t \mathbf{P}_q \) in Maxwell’s equations. Ultimately, the frequency range of the measured electrical current will be limited by both...
the measurement setup itself and the electrical properties of the device, such as its intrinsic capacitance.

4.1.1. Coherent Contribution

Using the Ehrenfest equation \( \dot{d}_i = i\hbar^{-1}[\{\hat{H}, \hat{d}_i\}] \), we can write the coherent part of the current density as

\[
J_{\text{coh}} = i\hbar n_{3D}q \{\hat{H}, \hat{d}_i\} \tag{49}
\]

In the following, we assume an effective mass Hamiltonian of the form \( \hat{H} = (1/2)p[m^*(\hat{r})]^{-1}\hat{p} + V(\hat{r}, t) \) as used in Equation (20), yielding

\[
J_{\text{coh}} = (1/2)n_{3D}q \left( \left[m^*(\hat{r}) \right]^{-1}\hat{p} + \hat{p}[m^*(\hat{r})]^{-1} \right) \tag{50}
\]

Using an orthonormal basis as for Equation (48), and inserting the unit operator \( \hat{I} = \int d^3r |r⟩⟨r| \) in Equation (50), we can express the result in terms of wavefunctions \( \varphi_i(r) = (r|i) \),

\[
J_{\text{coh}} = \hbar n_{3D}q \sum_{i,j} \langle \varphi_j | \rho_{jj} | \varphi_i | m^*(\hat{r})^{-1} \nabla \varphi_j(\hat{r}) \rangle d^3r \tag{51}
\]

Equation (51) can also be interpreted as the current density contribution of a representative individual (single-carrier) quantum system at the corresponding position, averaged over the associated volume \( V_\alpha = n_{3D}^{-1} \), where the microscopically resolved current density is given by the familiar expression\[94]\]

\[
J_{\text{coh}} = \hbar q \sum_{i,j} \langle \varphi_j | \rho_{jj} | m^*(\hat{r})^{-1} \nabla \varphi_j(\hat{r}) \rangle \tag{52}
\]

4.1.2. Incoherent Contribution

The incoherent current density is given by

\[
J_{\text{inc}} = n_{3D}q \langle \hat{N} \rangle_{\text{inc}} = n_{3D}q \text{Tr} \left[ \hat{r} \hat{d}_i | \text{inc} \right], \tag{53}
\]

which yields with Equations (3) and (4)

\[
J_{\text{inc}} = n_{3D}q \text{Tr} \left\{ i \sum_{k} \left( \hat{L}_k \hat{d}_i \hat{L}_k^\dagger - \frac{1}{2} \hat{d}_i \hat{L}_k^\dagger \hat{L}_k - \frac{1}{2} \hat{L}_k^\dagger \hat{L}_k \hat{d}_i \right) \right\} = n_{3D} \sum_{ij} \sum_{nm} D_{ijnm} \rho_{nm} \tag{53}
\]

For an incoherent transition from a state \( \alpha \) to \( \beta \neq \alpha \), we obtain with the corresponding Lindblad operator given in Equation (7)

\[
J_{\text{inc}}^{\alpha \rightarrow \beta} = r_{\alpha \rightarrow \beta} n_{3D} \left( \{d_{\beta\beta} - d_{\alpha\alpha}\} \rho_{\alpha\alpha} - \sum_{\gamma \neq \alpha} \Re \{d_{\alpha\gamma} \rho_{\gamma\gamma} \} \right) \tag{54}
\]

Furthermore, inserting Equation (12) in Equation (53) yields the pure dephasing contribution between two levels \( \alpha \) and \( \beta \)

\[
J_{\text{inc}}^{\alpha \beta} = -2\gamma_{\alpha \beta} n_{3D} \Re \{d_{\alpha\beta} \rho_{\beta\beta} \} \tag{55}
\]

with the pure dephasing rate \( \gamma_{\alpha \beta} \). The current contributions from incoherent transitions due to Equations (54) and (55) can also be rearranged so that

\[
J_{\text{hop}}^{\alpha \beta} = (r_{\alpha \rightarrow \beta} - r_{\beta \rightarrow \alpha}) n_{3D} \left( d_{\beta\beta} - d_{\alpha\alpha} \right) \tag{56}
\]

is the net current due to the hopping transport between states \( \alpha \) and \( \beta \) which corresponds to the classical rate equation description, and

\[
J_{\text{dep}}^{\alpha \beta} = -2\gamma_{\alpha \beta} n_{3D} \Re \{d_{\alpha\beta} \rho_{\beta\beta} \} \tag{57}
\]

is the dephasing contribution due to the decay of the corresponding off-diagonal matrix elements \( \rho_{\alpha \beta} \) and \( \rho_{\beta \alpha} \). Here, \( \gamma_{\alpha \beta} = (r_{\alpha} + r_{\beta})/2 + \gamma_{\alpha \beta} \) is the total dephasing rate, including lifetime broadening and pure dephasing, and \( r_{\alpha, \beta} \) is given by Equation (10). The total incoherent current density, resulting from incoherent transitions and pure dephasing, is then obtained by summing over all transitions. With Equations (56) and (57), we obtain

\[
J_{\text{inc}} = \sum_{\alpha=1}^{N-1} \sum_{\beta=\alpha+1}^{N} \left( J_{\text{hop}}^{\alpha \beta} + J_{\text{dep}}^{\alpha \beta} \right) = n_{3D} \sum_{\alpha} \sum_{\beta \neq \alpha} \{ r_{\alpha \rightarrow \beta} - r_{\beta \rightarrow \alpha} \} \left( d_{\beta\beta} - d_{\alpha\alpha} \right) - \gamma_{\alpha \beta} n_{3D} \Re \{d_{\alpha\beta} \rho_{\beta\beta} \} \tag{58}
\]

4.2. Slowly Varying Amplitude Approximation

Although the Bloch equations in RWA, Equation (43), are sometimes solved in combination with the full Maxwell’s equations, Equation (44), typically the RWA is combined with an envelope propagation equation, derived from Maxwell’s equations under the assumption of a slowly varying field amplitude. In this way, above mentioned advantages of the RWA, namely a significantly reduced numerical burden and a larger number of analytical solutions, also applies to the coupled Maxwell–Bloch system. Taking the curl of Equation (44a) and eliminating \( \mathbf{H} \) using Equation (44b) yields

\[
\nabla \times \nabla \times \mathbf{E} = -\frac{n_0^2(1 - 2\Delta_s)}{c^2} \mathbf{E} - \mu_0 \sigma \mathbf{J} - \mu_0 \mathbf{d} \mathbf{E} - \mu_0 \mathbf{d} \mathbf{J} = \mu_0 \mathbf{d} \mathbf{P} \tag{59}
\]

Here, \( \epsilon = (\mu_0 \epsilon_0)^{-1/2} \) is the vacuum speed of light. Furthermore, the background permittivity of the host material \( \epsilon_i(\mathbf{x}) \) is here modeled as \( \epsilon_i = n_0^2(1 - 2\Delta_s) \), where \( \Delta_s(x, y) \) (with the minimum value 0) describes a transverse refractive index profile, as widely employed in waveguiding structures.[109]

For no free space charges, Gauss’s law dictates that \( \nabla \cdot \mathbf{D} = 0 \) where \( \mathbf{D} = p_0 + \epsilon_0 n_0^2(1 - 2\Delta_s) \mathbf{E} \) is the displacement field in Equation (59). Assuming an isotropic medium, we can thus set \( \nabla \cdot \mathbf{V} \approx 0 \) in the case of weak nonlinearity[157] and weak inhomogeneity.[109,170] or generally if the field intensity transverse to the propagation direction is slowly varying over an optical wavelength.[171] This assumption is only fulfilled for weak waveguiding, that is, if the relative changes of the refractive index \( |\Delta n_s|/n_0 \) and its gradient \( |\Delta(\nabla n_s)|/|\nabla n_0| \) over the distance of a
wavelength in the medium is small against unity,\(^{[169]}\) where \(n_0 = n_0(1 - 2\Delta_n)/2\) in Equation (59). Furthermore, also the polarization contribution \(P_q\) of the quantum structure must be compatible with the assumption of weak inhomogeneity. As discussed in Section 3.3, quantum structures, as modeled by the Bloch equations, can be highly anisotropic; for example, the dipole moment element vector \(d_i\) of inter-conduction band transitions in quantum wells only has a nonzero component in growth direction. If the optical field is however also polarized in this direction, which is, for example, often the case in lasers since only the corresponding field component gets amplified, then \(V \approx 0\) can still hold for weak nonlinearity and inhomogeneity. Using \(V(x \times E) = V(\nabla E) - \nabla^2 E\) and subsequently neglecting the term \(V(\nabla E)\), we obtain the generalized inhomogeneous wave equation

\[
\nabla^2 E = \frac{n_0^2(1 - 2\Delta_n)}{c^2} \partial_t^2 E + \mu_0 \sigma \partial_t E + \mu_0 \partial_t J_f + \mu_0 \partial_t^2 P_q
\]

For deriving the slowly varying amplitude approximation (SVAA), \(E\) and \(P_q\) are written as a product of its envelope and carrier, as done above for the derivation of the RWA. However, in contrast to Equation (41), we also take into account the spatial dependence of the carrier, where we assume that the direction of the optical energy flow at every position is close to a reference direction defined by the carrier wavevector \(k_c\), which corresponds to the paraxial approximation. This assumption is, for example, typically fulfilled in laser resonators or optical fibers. Introducing the complex-valued field and polarization amplitudes, \(\mathbf{E}(x, t)\) and \(\mathbf{P}(x, t)\), and assuming propagation along the \(z\) direction, we have

\[
\mathbf{E}(x, t) = \frac{1}{2} \mathbf{E}(x, t) \exp(ikxc) + \text{c.c.}
\]

\[
\mathbf{P}(x, t) = \frac{1}{2} \mathbf{P}(x, t) \exp(ikxc) + \text{c.c.}
\]

with \(|k_c| = n_0\omega/c\). We note that although Equation (61a) contains the term \(\exp(ikzc)\) not included in Equation (41), the Bloch equations in RWA, Equation (43), remain unchanged since \(\exp(ikzc)\) cancels out. To apply the SVAA, we insert Equation (61) in Equation (60). Just as for the RWA, we assume that all significant spectral components of the field are close to \(\omega_c\) that is, at frequencies \(\omega_c + \Delta_\omega\) with \(|\Delta_\omega| \ll \omega_c\). This implies that \(\partial_t^2 E\) can be neglected against \(-2\omega_c \partial_t E\), as can be seen in Fourier domain where the two terms become \(-\Delta_\omega \partial_t E(\Delta_\omega)\) and \(-2\omega_c \Delta_\omega \partial_t E(\Delta_\omega)\). Similarly, also \(\sigma \partial_t E\) and \(\Delta_\omega \partial_t E\) can be dropped against \(-\omega_c \sigma E\) and \(-\omega_c \Delta_\omega E\). The polarization amplitude \(\mathbf{P}\), introduced in Equation (61b), couples the optical propagation equation to the Bloch equations, Equation (43), as further discussed in Section 4.2.1. The RWA implies that also \(\mathbf{P}\) is narrowband, which means that, for example, harmonic or difference frequency generation cannot be included. Thus, similarly as for the field, \(\partial_t^2 \mathbf{P}\) and \(-2i\omega_c \partial_t \mathbf{P}\) can be neglected against \(-\omega_c^2 \mathbf{P}\). In addition, the paraxial approximation implies that \(\partial_t E\) can be neglected against \(ik_c \partial_x E\). Finally, multiplying all terms with \(\exp(i\omega_c t - ikzc)\) and discarding all rapidly oscillating terms, which also eliminates \(J_f\) since it is assumed to contain only low frequency components (see Section 4.1), we arrive at

\[
\dot{\partial}_t E = \frac{\mu_0}{n_0} \partial_t E = -i\omega_c \Delta_\omega E + \frac{1}{2n_0^2} \left(\frac{i\omega_c}{\epsilon_0} \nabla^2 E + \frac{\omega_c}{\epsilon_0} \mathbf{P} - \sigma E\right)
\]

(62)

Here, \(\nabla^2 = \partial_x^2 + \partial_y^2\) denotes the transverse Laplace operator. The “+” and “−” signs in Equation (62) are for forward and backward propagation corresponding to \(k_c > 0\) and \(k_c < 0\), respectively. For counterpropagating fields which, for example, arise in Fabry–Pérot resonators, the standing wave pattern causes a position dependent inversion grating, also referred to as spatial hole burning. This effect is not yet included in Equation (62), and its implementation is discussed in Section 5.3.2.

4.2.1. Polarization in Rotating Wave Approximation

In the RWA, the off-diagonal density matrix elements \(\rho_{ij}\) that are associated with near-resonant optical transitions are represented in terms of transformed elements \(\rho_{ij}\) in a rotating reference frame, as obtained with Equation (42). Writing the total current as \(J_q = J_f + \partial_t P_q\) as in Equation (47), and assigning the low-frequency contributions to \(J_i\) and the optical contributions to \(P_q\), we see from Equation (48) that the transformation into the rotating frame only affects the evolution of the polarization \(P_q\). With Equations (46) and (42), we obtain

\[
P_q = n_{3D} \sum_{\omega > 0} \mathbf{d}_{ij} \eta_{ij} \exp(-i\omega_c t) + \text{c.c.} + n_{3D} \sum_{\omega > 0} \mathbf{d}_{ij} \rho_{ij}
\]

(63)

For inclusion of optical propagation, the RWA is often not coupled to the full Maxwell equations, but rather solved together with Equation (62) in SVAA which contains the polarization in terms of the amplitude \(\mathbf{P}\). As discussed above, we have to replace \(\exp(-i\omega_c t)\) by \(\exp(i\omega_c t)\) in Equation (63) since the SVAA also takes into account the spatial dependence of the carrier. Comparing the resulting equation with Equation (61b), and neglecting the quasi-static dipole moment contribution \(\sum_{\omega > 0} \mathbf{d}_{ij} \rho_{ij}\) which does not oscillate at the optical excitation frequency and thus drops out in the SVAA, we obtain

\[
\mathbf{P} = 2n_{3D} \sum_{\omega > 0} \mathbf{d}_{ij} \eta_{ij}
\]

(64)

4.3. Initial Conditions

The Bloch equations without or with RWA, Equation (17) or (43), have to be supplemented by corresponding initial conditions at time \(t = t_0\). Apart from special cases where the quantum system may be coherently prepared in a certain initial state such as a coherent superposition,\(^{[172]}\) the system will be initially in equilibrium. The corresponding density matrix elements are then obtained by setting \(\dot{\rho}_{ij} = 0\) in Equation (17) or (43) and assuming a vanishing optical field for \(t \leq t_0\), which gives rise to a mixed state with off-diagonal elements \(\rho_{ij}(t = t_0) = 0\) and \(\eta_{ij}(t = t_0) = 0\), respectively. The diagonal elements \(\rho_{ii}(t = t_0) = \rho_{ii}^{eq}\) are given by the equilibrium occupation probabilities \(\rho_{ii}^{eq}\), which can be
obtained by setting $d_i = 0$ in Equation (9). This yields for a system with $N$ levels the linear equation system

$$0 = \sum_{j \neq i} r_{j \rightarrow i} \rho_{ji}^{eq} - r_{i \rightarrow j} \rho_{ij}^{eq}, \quad i = 1, \ldots, (N - 1)$$

$$1 = \sum_{i=1}^{N} \rho_{ii}^{eq}$$

(65) \hspace{1cm} (66)

where $r_i$ is given by Equation (10). The $\rho_{ii}^{eq}$ do not necessarily correspond to a thermal distribution, but are rather determined by the transition rates which may, for example, include the pumping process in lasers. For inhomogeneous device structures, the rates $r_i$ and $r_{j \rightarrow i}$ generally depend on position $x$, giving rise to $x$ dependent $\rho_{ij}^{eq}$.

Suitable initial conditions also have to be defined for the Maxwell equations, Equation (44), or the propagation equations in SVA derived thereof, Equation (62). Here, we cannot choose identically vanishing fields, since the optical field would then remain zero throughout the MB simulation. Laser seeding by spontaneous emission is often mimicked by initializing the electric field with white Gaussian amplitude noise, which can also be added at every time step of the simulation to model spontaneous emission noise. For a real-valued, redundancy-free representation can be obtained by applying Equations (27) and (28), yielding the three real-valued quantities $w := \langle \dot{u} \rangle_{12} = \rho_{12} + \rho_{21} = 2 \Re \{ \rho_{21} \}$, and $w := \langle \dot{v} \rangle_{12} = -i(\rho_{12} - \rho_{21}) = -2 \Im \{ \rho_{21} \}$, and $w := \langle \dot{v} \rangle_{12} = \rho_{22} - \rho_{11}$. These are usually represented in terms of the so-called Bloch vector $S = [u, v, w]^T$, where a minus sign has been added to the definition of $v$ in order to obtain the usual convention for the Bloch vector. \cite{49} Separating $\Omega$ in its real and imaginary part $\Omega_+ + i \Omega_-$, Equation (67) then becomes

$$\partial_t u = -\omega_{21} v + 2\Omega_+ w - \gamma_2 u$$

$$\partial_t v = \omega_{21} u + 2\Omega_+ w - \gamma_2 v$$

$$\partial_t w = -2\Omega_- u - 2\Omega_- v - \gamma_1 w + \Gamma_{12}$$

(69a) \hspace{1cm} (69b) \hspace{1cm} (69c)

which can also be written as \cite{49}

$$\partial_t S = \begin{pmatrix}
-2\Omega_+ v \\
2\Omega_+ v \\
\gamma_1 (w - w_{eq})
\end{pmatrix}$$

(70)

The polarization term in Equation (44) is then with Equation (48) obtained as

$$\partial_t P_q = 2n_{32} \Re \{ d_{12} \partial_t \rho_{21} \}$$

$$= n_{32} \Re \{ d_{12} \partial_t u + \Re \{ d_{12} \} \partial_t v \}$$

(71)

The time evolution of the Bloch vector $S(t)$ can be visualized in the Bloch sphere representation, where the Bloch vector trajectory is displayed in a Cartesian coordinate system with axes $u$, $v$, and $w$. For pure states, $|S(t)| = 1$, that is, the tip of the Bloch vector moves along the surface of a unit sphere, the so-called Bloch sphere. For mixed states, the tip is located within the Bloch sphere, corresponding to $|S(t)| < 1$. In Figure 7, the time evolution of the Bloch vector components and the corresponding Bloch vector trajectory are shown for a two-level system with $\gamma_1 = \gamma_2 = 0$ and initial conditions $u = v = 0$, $w = -1$. The optical field is assumed to be a sech pulse $\Omega = 2T^{-1} \text{sech}(t/T)$, which corresponds to a self-induced transparency soliton as further discussed in Section 6.1.2, with $T = 10/\omega_{01}$ chosen for this example.

A further representation of the Bloch equations is obtained by assuming a real $d_{12}$ and thus $\Omega = \Omega_+$. Solving Equation (69a) for $v$ and using the result to eliminate $v$ in Equations (69b) and (69c) yields with Equation (71)\cite{52}

$$\partial_t P_q + 2\rho_{21} \partial_t \rho_{21} + \omega_{21} \rho_{21} + \gamma_1 \rho_{21} = -\frac{2\omega_{21} d_{12}^2}{\hbar} n_{32} w \Re \frac{d_{12}}{d_{12}}$$

(72a)

$$\partial_t w = \frac{2}{\hbar n_{32}} \partial_t \rho_{21} + \gamma_1 \rho_{21} - \gamma_1 w + \Gamma_{12}$$

(72b)

This representation can be seen as an extension of the classical Lorentz model for resonant polarization in dielectrics, assuming the same mathematical form as Equation (72a) if we set $w$ constant. Accordingly, Equation (72) is mainly used in computational electrodynamics, especially in combination with the finite-difference time-domain method, as a substitute for more basic classical polarization models.\cite{52}
4.4.1. Rotating Wave/Slowly Varying Amplitude Approximation

In the RWA, we obtain from Equation (43) with \( \Omega = \hbar^{-1} d_{21} \Phi \)
\[
\begin{align*}
\partial_t \eta_{21} &= i \Delta \eta_{21} - \frac{1}{2} i u \Omega - \gamma_{2} \eta_{21} \quad (73a) \\
\partial_t w &= i (n^*_{21} \Omega - \eta_{21} \Omega^*) - \gamma_1 (w - w_{eq}) \quad (73b)
\end{align*}
\]
where \( \Delta = \omega_1 - \omega_{21} \) denotes the detuning of the optical field from the resonance frequency \( \omega_{21} \). In analogy to above, we can introduce the Bloch vector \( s \) for the off-diagonal density matrix elements in RWA, with components \( s_1 = \eta_{12} + \eta_{21} = 2 \Re\{\eta_{21}\} \), \( s_2 = -i(\eta_{12} - \eta_{21}) = -2 \Im\{\eta_{21}\} \), \( s_3 = w \), and obtain in analogy to Equation (69) with \( \Omega = \Omega_r + i \Omega_i \)
\[
\begin{align*}
\partial_t s_1 &= \Delta s_2 + \Omega w - \gamma_2 s_1 \quad (74a) \\
\partial_t s_2 &= -\Delta s_1 + \Omega w - \gamma_2 s_2 \quad (74b) \\
\partial_t w &= -\Omega s_1 - \Omega s_2 - \gamma_1 (w - w_{eq}) \quad (74c)
\end{align*}
\]

The polarization term in the SVAA propagation equation, Equation (62), is then with Equation (64) obtained as
\[
P = 2n_{3D} d_{12} \eta_{21} = n_{3D} d_{12} (s_1 - is_2) \quad (75)
\]

5. Reduction to 1D Model

Although the MB equations are sometimes solved in two or even three spatial dimensions,\(^{[53-60]}\) the model is frequently reduced to a single spatial coordinate in order to minimize the numerical load.\(^{[98]}\) This is usually achieved by assuming plane wave propagation in the Maxwell equations, Equation (44), or the corresponding propagation equations in SVAA, Equation (62).\(^{[174]}\) For extended beams propagating in a homogeneous medium such as a gas or bulk solid-state medium, the plane wave approximation may be a reasonable assumption. For optoelectronic devices which are the focus of this paper, the light is usually strongly guided, often with sub-wavelength confinement in at least one dimension. Here, the plane wave approximation is clearly too simplistic. However, optoelectronic devices such as semiconductor-based lasers often employ waveguiding structures which are invariant in propagation direction \( z \), in particular, schemes with a suitable transverse refractive index profile or metal cladding. Such geometries provide lateral field confinement and give rise to guided mode solutions, that is, field solutions which are at a given frequency \( \omega \) characterized by a propagation constant and a \( z \) independent transverse field distribution. While some 1D plane wave treatments have included all transverse field components to describe elliptically or circularly polarized light,\(^{[152,153,175-177]}\) we assume linearly polarized waveguide modes in the following, and thus consider a single transverse component of the electric and magnetic fields. In Figure 8, an exemplary waveguide structure is schematically illustrated.

5.1. Full Maxwell Equations

We employ the full Maxwell equations, Equation (44), coupled to the Bloch equations, Equation (16) or (17), to describe the carrier–light interaction and optical propagation in a waveguide...
geometry which is invariant with respect to the propagation direction \( z \). Our goal is to extract a 1D MB model with a single electric and magnetic field component, as typically used in simulations due to the associated computational burden. We focus on guided mode solutions, which are at a given frequency \( \omega \) characterized by a (generally complex) propagation constant \( \beta \) and \( z \) invariant transverse field dependencies \( E_{y,z}(x, y) \) and \( H_{y,z}(x, y) \) for the electric and magnetic field components. Thus, we can make the ansatz

\[
E_p(x, t) = \Re \left\{ E_p(x, y) \exp \left( i \beta z - i \omega t \right) \right\} = \Re \left\{ E_p^\omega(x) \exp \left( -i \omega t \right) \right\}
\]

(76a)

\[
H_p(x, t) = \Re \left\{ H_p(x, y) \exp \left( i \beta z - i \omega t \right) \right\} = \Re \left\{ H_p^\omega(x) \exp \left( -i \omega t \right) \right\}
\]

(76b)

with \( p = x, y, z \). By inserting Equation (76) into Equation (44), the computation of the transverse mode profile in the xy-plane can be decoupled from the \( z \) coordinate and reduces to a 2D problem. For example, by eliminating the electric field, we obtain

\[
(\partial_x^2 + \partial_y^2) H^\omega_p + \frac{i \epsilon_p}{\epsilon_0} (\partial_y H^\omega_p - \partial_x H^\omega_y) = \left( \beta^2 - \frac{\omega^2}{c^2} \epsilon_0 \right) H^\omega_p
\]

(77)

with \( p = x, y \) and \( q = y, x \).[178] Waveguiding is, for instance, obtained by surrounding the optically active region with another dielectric material featuring a lower refractive index as illustrated in Figure 8b, or with a metal cladding. Both cases can be described by a transversely dependent complex background permittivity

\[
\epsilon_p = \epsilon_I + \sigma / (i \omega \epsilon_0)
\]

(78)

where \( \epsilon_I \) and \( \sigma \) generally depend on \( x, y \), and \( \omega \), and \( \sigma \) accounts for the conductivity or dielectric losses. Together with the boundary condition \( H^\omega_p \rightarrow 0 \) for \( x^2 + y^2 \rightarrow \infty \), Equation (77) constitutes a complex eigenvalue problem. Equation (77) can, for example, be solved with the film mode matching method, which is especially suitable for waveguides with a rectangular cross section.[178] The polarization contribution \( P_q \) in Equation (44) due to the quantum systems is not yet considered in Equation (77) since it is assumed to be small enough to be included in first-order perturbation theory, with negligible influence on the transverse field distribution. Using \( \nabla \mathbf{H} = 0 \), we can calculate the longitudinal component \( H^\omega_p(x, y) \) from \( H^\omega_x \) and \( H^\omega_y \) as

\[
H^\omega_p = i \beta^{-1} (\partial_x H^\omega_x + \partial_y H^\omega_y)
\]

(79)

Furthermore, the electric field components are with Equation (44b) obtained as

\[
\omega \sigma \epsilon_p E_{p}^\omega = i \beta \left( H^\omega_p + \beta H^\omega_x \right)
\]

(80a)

\[
\omega \sigma \epsilon_p E_{p}^\omega = -\beta H^\omega_y - i \partial_y H^\omega_y
\]

(80b)

\[
\omega \sigma \epsilon_p E_{p}^\omega = i \beta H^\omega_x - i \partial_x H^\omega_y
\]

(80c)

For general solutions of Equation (77), the polarization varies over the waveguide cross section. As indicated in Figure 8b, in many optoelectronic devices, such as typical standard edge-emitting and quantum cascade lasers, rectangular waveguides are used where the width in lateral \( y \) direction significantly exceeds its thickness in \( x \) direction. This allows an approximate treatment as a slab waveguide structure, which is assumed to be infinitely extended in \( y \) direction and thus can, to first order, be described by \( E_p(x) \). The field components are then assumed to be constant in \( y \) direction, which corresponds to setting \( \partial_y = 0 \).[170]

The guided field solutions can be divided into two classes: transverse electric (TE) modes are characterized by \( E^\omega = 0 \), where for \( \partial_y = 0 \) all components except \( H^\omega_x \), \( E^\omega_y \), and \( H^\omega_y \) vanish as can be seen from Equations (79) and (80); similarly, transverse magnetic (TM) modes, characterized by \( H^\omega_y = 0 \), have for \( \partial_y = 0 \) only non-vanishing \( H^\omega_x \), \( E^\omega_y \), and \( E^\omega_z \) components.[170] The \( y \) dependence of the field distribution may then be reintroduced using the effective refractive index approximation method,[180] which preserves the TE or TM character of the solution. From the discussion of dipole matrix elements for quantum well structures in Section 3.3, it follows that standard edge-emitting lasers, which utilize interband transitions, preferentially operate in TE mode (see also Figure 5a). On the other hand, QCLs, which rely on intraband transitions, only operate in TM mode (see also Figure 5c).

As pointed out above, simulations typically employ a plane-wave-type propagation model which only depends on the propagation coordinate \( z \) and time \( t \), and considers a single transverse electric and transverse magnetic field component. Our goal is to derive such equations, with a form equivalent to the Maxwell equations, for guided rather than plane-wave propagation, as applies to many photonic devices and systems.

### 5.1.1. Transverse Electric Mode

For TE modes in slab waveguides, Equation (77) yields with \( H^\omega_y = 0 \) and \( \partial_y = 0 \)

\[
\partial_x H^\omega_x = \left( \beta^2 - \frac{\omega^2}{c^2} \epsilon_0 \right) H^\omega_x
\]

(81)

and the boundary conditions are given by \( H^\omega_x(x \rightarrow \pm \infty) \rightarrow 0 \). From Equation (44), we furthermore obtain

\[
-\partial_x E_x = -\mu_0 \partial_x H_x
\]

(82a)

\[
\partial_x H_x - \partial_x H_z = \epsilon_0 \epsilon_I \partial_y E_y + \sigma E_y
\]

(82b)

The polarization contribution of the quantum systems is not contained in Equation (82b) since it will subsequently be included in a perturbative manner. Equation (82b) does not yet have the desired form since it contains an \( x \) derivative and the longitudinal field component in the term \( \partial_x H_z \). With Equations (76b), (79), and (81), we obtain

\[
\partial_x H^\omega_x = i \beta^{-1} \left( \beta^2 - \frac{\omega^2}{c^2} \epsilon_0 \right) H^\omega_x
\]

(83)
where \( \varepsilon_r = \varepsilon_r + i \sigma / (\omega \varepsilon_0) \). In the following, it is practical to switch to the frequency domain, where Equation (82a) is with Equation (76) given by

\[
\partial_t E_v = i \beta E_v = -i \omega \mu_0 H_z^c
\] (84)

From Equation (84), we see that the electric and magnetic fields have the same transverse distribution. Inserting Equation (83) into Equation (82b) in frequency domain, and employing Equation (84), we arrive at

\[
\partial_z H_z^c = -i \omega \mu_0 \beta^2 E_v^c
\] (85)

In the following, the polarization contribution of the quantum system will be included as a perturbation.\(^{(181)}\) Re-deriving Equation (81) from Maxwell’s equations, Equation (44), but now with the polarization contribution due to the quantum systems included, we see that the perturbation generated by the polarization on the \( E_v^c \) field component is formally equivalent to an additional background permittivity \( \Delta \varepsilon_r = \varepsilon_r - P_v^c / E_v^c \), where \( P_v^c \) contains the polarization contribution of the quantum systems in frequency domain. In the following, we assume that the device operates in a single transverse mode with the magnetic field distribution \( H_z^c \), possibly the fundamental mode. Using the similarity of Equation (81) to the Schrödinger equation in quantum mechanics, we can apply perturbation theory in an analogous manner.\(^{(182)}\) To first order, \( H_z^c \) remains unchanged, and for the eigenvalue \( \beta^2 \) we obtain the correction

\[
\Delta \beta^2 = \frac{\omega^2}{\varepsilon_0 E_v^c c^2} \int_{-\infty}^{\infty} \left| H_z^c \right|^2 P_v^c dxdy \] (86)

For completeness, we also include integration over the \( y \) coordinate in Equation (86) since the \( y \) dependence of \( H_z^c \) may be reintroduced based on the above mentioned effective refractive index method. It should be mentioned that if \( \varepsilon_r \) in Equation (81) has a nonvanishing imaginary part, the eigenvalue problem is non-Hermitian and strictly speaking, a biorthogonal basis set must be used.\(^{(183)}\) In this case, Equation (86) serves as an approximation to the unperturbed equations. Furthermore, it is practical to split the unperturbed propagation constant \( \beta \) into a real and an imaginary part, \( \beta = \beta^* + i \beta' \). Here, \( \beta^* \) is related to the power loss coefficient \( a \) by \( \beta^* = \text{sgn}(\beta) a / 2 \), with the sign function \( \text{sgn} \). Assuming \( |\beta| \gg |\beta^*| \), we can write \( \beta^2 \approx \beta^* + i a + \Delta \beta^2 \). Introducing the effective waveguide refractive index \( n_{\text{eff}}(\omega) \) defined by \( \beta = \text{sgn}(\beta) \omega n_{\text{eff}} / c \), we then obtain

\[
\partial_z H_z^c = -i \omega n_{\text{eff}}^2 H_z^c + \varepsilon_0 n_{\text{eff}} \partial_t E_v^c = -i \omega n_{\text{eff}} \int_{-\infty}^{\infty} \left| H_z^c \right|^2 P_v^c dxdy \int_{-\infty}^{\infty} \left| H_z^c \right|^2 dxdy
\] (87)

Field Confinement Factor: Equations (84) and (87) effectively reduce the complexity of the propagation problem from three spatial dimensions to a single coordinate \( z \). However, for computing the integral in the polarization term of Equation (87), \( P_v^c \) must be obtained by solving the Bloch equations in the whole device volume, using the full spatial field dependence given by Equation (76). This greatly impedes the numerical efficiency of the 1D propagation model. As indicated in Figure 8a, frequently the transverse field distribution does not vary significantly across the quantum nanostructure, for example, because the nanostructure covers only part of the waveguide cross section, preferably at the position of maximum intensity. Consequently, also \( P_v^c \) is approximately constant over the quantum system cross section and can be taken out of the integral in Equation (86), which can then be written as \( \Gamma P_v^c \). Here, \( \Gamma \) denotes the field confinement factor, which gives the overlap of the quantum nanostructure with the mode profile and is thus also referred to as overlap factor. With Equation (84), \( \Gamma \) can be written as

\[
\Gamma = \frac{\int_{-\infty}^{\infty} \left| H_z^c \right|^2 dxdy}{\int_{-\infty}^{\infty} \left| H_z^c \right|^2 dxdy} = \frac{\int_{-\infty}^{\infty} \left| E_v^c \right|^2 dxdy}{\int_{-\infty}^{\infty} \left| E_v^c \right|^2 dxdy}
\] (88)

Here, the numerator contains an integration over the cross-sectional area \( A_y \) of the active region formed by the quantum systems. The intensity distribution in the waveguide is given by the time-averaged magnitude of the \( z \) component of the Poynting vector, which is, with Equation (84), obtained as

\[
I = \langle |S_z| \rangle = \left| \langle \hat{H}_z^c (\hat{H}_x^c)^* \rangle \right| / 2 = \varepsilon_0 \omega n_{\text{eff}} \langle |E_v^c| \rangle^2 / 2
\] (89)

With Equations (84) and (88), we then arrive at the usual definition\(^{(184)}\)

\[
\Gamma = \frac{\int_{-\infty}^{\infty} \langle |S_z| \rangle dxdy}{\int_{-\infty}^{\infty} \langle |S_z| \rangle dxdy}
\] (90)

The meaning of \( \Gamma \) is visualized in Figure 9. We can represent the field confinement factor as \( \Gamma = A_y / A_{\text{eff}} \), where \( A_{\text{eff}} \) is the area covered by an equivalent mode which conserves \( \int_{-\infty}^{\infty} \langle |S_z| \rangle dxdy \), but has a rectangular intensity distribution with \( \langle |S_z| \rangle \) fixed to the value in the quantum nanostructure. Thus, the optical power can with Equation (89) be written as

\[
P = |I| A_{\text{eff}} = \left| \left( E_v^c \right)_0 \right|^2 A_{\text{eff}} \varepsilon_0 \omega n_{\text{eff}} / 2
\] (91)

where \(|I|\) and \( \left| E_v^c \right|_0 \) refer to the values of \( I \) and \( E_v^c \) in the quantum nanostructure.

1D Maxwell Equations: In the following, we regard the \( E_v^c \) and \( H_z^c \) fields at a frequency \( \omega \) as spectral components of time-dependent fields \( E_y \) and \( H_z \), and transform Equation (87) into time
domain. For convenience, we do not consider the \( \omega \) dependence of \( E_{\omega}^{x} \) and \( H_{\omega}^{x} \) in Equation (88), but rather evaluate \( \Gamma \) at the center frequency \( \omega_0 \) of the optical field. Furthermore, to obtain a form compatible with Equation (82b), we divide \( n_{\text{eff}}^{2}(\omega_0) \) into a constant part, for example, the value \( n_{\text{eff}}^{2}(\omega_0) \) at \( \omega = \omega_0 \), and a frequency dependent part \( \Delta\varepsilon_{\text{eff}} = n_{\text{eff}}^{2}(\omega) - n_{\text{eff}}^{2}(\omega_0) \) which describes chromatic waveguide dispersion and gives rise to an extra polarization contribution. Considering that multiplications with \( \omega \) in frequency domain correspond to operators \( i\omega \) in time domain, we obtain from Equations (84), (87), and (48)

\[
\partial_t E_{y} = \mu_0 \partial_x H_{y} \quad \text{(92a)}
\]

\[
\partial_t H_{y} = \varepsilon_0 n_{\text{eff}}^{2}(\omega_0) \partial_x E_{y} + \sigma (i\omega) E_{y} + \Gamma n_{1D} \sum_{i, j} d_{i, j} \partial_{\rho_{ij}} + \varepsilon_0 \partial_x [\Delta\varepsilon_{\text{eff}}(i\omega) E_{y}] \quad \text{(92b)}
\]

Here, the generally frequency dependent conductivity

\[
\sigma(\omega) = \varepsilon_0 n_{\text{eff}}^{2}(\omega_0) \sigma(\omega_0)
\]

is often approximated by \( \sigma = \sigma(\omega_0) \). Obviously, \( \Delta\varepsilon_{\text{eff}} \) and \( \sigma \) must be even functions \( f(-\omega) = f(\omega) \) to preserve the real-valued character of Equation (92). Furthermore, causality requires that the real and imaginary parts of the complex permittivity defined in Equation (78) fulfill the Kramers–Kronig relation, which is, strictly speaking, already violated when modeling a medium as a lossless, frequency independent dielectric with \( \varepsilon_r \neq 1 \).

Notably Equation (92) does not explicitly depend on \( x \) and \( y \) anymore. Thus, it is practical to identify \( H_{z}(z, t) \) and \( E_{y}(z, t) \) with the field strengths at the transverse position of the nanostructure, because then \( E_{y} \) can directly be used in Equation (16) or (17) to evaluate \( \partial_{\rho_{ij}}(z, t) \). For completeness, we mention that the longitudinal magnetic field component \( H_{x} \) can be obtained from \( \nabla \mathbf{H} = 0 \), that is, \( \partial_y H_x = -\partial_x H_y \).

### 5.1.2. Transverse Magnetic Mode

For TM modes in slab waveguides, Equation (77) yields with \( H_{z}^{0} = 0 \) and \( \partial_y = 0 \)

\[
\varepsilon_x \partial_x \left( \varepsilon_x^{-1} \partial_x H_{y}^{0} \right) = \left( \beta_{y}^{2} - \frac{\omega^2}{c^2} \varepsilon_x \right) H_{y}^{0} \quad \text{(94)}
\]

and the boundary conditions are given by \( H_{y}^{0}(x \to \pm \infty) \to 0 \). The mutual dependence of the field components is given by Equation (80), which yields with Equation (76)

\[
\varepsilon_{y} \varepsilon_{y} \varepsilon_{x} \varepsilon_{x}^{*} = \partial_y H_{y}^{0} = i\beta_{y} H_{y}^{0} \quad \text{(95)}
\]

\[
\varepsilon_{y} \varepsilon_{y} \varepsilon_{x} \varepsilon_{x}^{*} = -\partial_y H_{y}^{0} \quad \text{(96)}
\]

From Equation (44a), we furthermore obtain with Equation (76)

\[
\partial_y E_{x}^{0} = i\omega \mu_0 H_{y}^{0} + \partial_x E_{x}^{0} \quad \text{(97)}
\]

Using Equation (96) to eliminate \( E_{x}^{0} \) in Equation (97) yields with Equation (94)

\[
\partial_y E_{x}^{0} = \frac{i}{\omega \varepsilon_0 \varepsilon_{y} \varepsilon_{x}} \beta_{y}^{2} H_{y}^{0} \quad \text{(98)}
\]

In Figure 10, the fundamental TM mode of a QCL waveguide structure is shown. The magnetic field distribution \( H_{y}^{0} \) is continuous, while \( E_{x}^{0} \) exhibits jumps at interfaces of layers with different \( \varepsilon_{y} \), as can also be seen from Equation (95).

In the following, we treat the background refractive index \( n_0 \) of the host material for the quantum systems as a real constant, assuming that the main frequency dependence and gain/loss in the nanostructure is provided by the quantum systems rather than the host material. Furthermore, although, for example, in a quantum well structure the barrier and well materials will have different refractive indices as indicated in Figures 8b and 9, the nanostructured region can still be approximately described by a single effective \( \varepsilon_{y} \) since the individual layers are too thin to be resolved by the optical field. For TM modes, the effective permittivity is then obtained as the harmonic mean of the individual permittivity values, that is, we obtain in the host material

\[
\varepsilon_{y}^{*} = (\Delta_{1}\varepsilon_{y}^{*} + \Delta_{2}\varepsilon_{y}^{*})/(\Delta_{1} + \Delta_{2}) \quad \text{where} \quad \Delta_{i} = \varepsilon_{i} - \varepsilon_{0}^{*}
\]

The total thicknesses and permittivites of the regions made from material \( i = 1, 2 \).

Generally, the treatment of TM modes is known to be more complex than for TE modes. Specifically, in contrast to the TE case, the derivation of 1D Maxwell-type equations for the transverse field components is not as straightforward as in Section 5.1.1. This can, for example, be seen from Equation (97), which only assumes a Maxwell-type form in analogy to Equation (92a) if \( \partial_y E_{x}^{0} \) can be neglected. Similarly as in Section 5.1.1, we assume that the fields are approximately constant over the transverse cross section of the nanostructured region, and identify in the following \( E_{x}^{0} \) and \( H_{y}^{0} \) with the field strengths at the transverse position of the nanostructure. With \( \varepsilon_{x} = n_0^2 \), we obtain from Equation (98)
\[ \partial_t E^w = i \omega \mu_0 n_{\text{eff}}^2(\omega) \frac{n_0^2}{n_0^2} \frac{H^w}{\epsilon_0} \]  

(99)

where we have assumed that \( |\beta'| < |\beta| \) and approximated \( \beta^2 \approx \beta^2 = n_{\text{eff}}^2 c^2 / \epsilon_0 \). Furthermore, we have neglected the frequency dependence of \( n_{\text{eff}} \), evaluating it at the center frequency \( \omega = \omega_c \). Of the optical field, so as to formally obtain a Maxwell-type equation with a frequency independent effective relative permittivity \( \epsilon_{\text{eff}} = n_{\text{eff}}^2(\omega)/n_0^2 \). In order to complete our model, Equation (99) must be complemented by a second Maxwell-type equation with a form similar to Equation (85) in frequency domain, that is, Equation (92b) in time domain. Importantly, this equation has to include the losses and frequency dependence omitted in Equation (99), so that the correct field propagation dynamics is obtained. Specifically, from Equation (76), we obtain the field propagation equations in frequency domain \( \partial_t E^w = -\beta^2 E^w, \partial_t H^w = -\beta^2 H^w \). This requires that

\[ \partial_t H^w = i \frac{n_0^2}{\omega \mu_0 n_{\text{eff}}^2(\omega)} \beta^2 E^w \]  

(100)

as can be verified by differentiating Equation (99) with respect to \( z \) and eliminating \( H^w \) with Equation (100), or alternatively eliminating \( E^w \) in an analogous way.

As in Section 5.1.1, the polarization due to the quantum systems is again perturbatively included in terms of a change \( \Delta \beta^2 \) to \( \beta^2 \). To this end, we re-derive Equation (94) from Maxwell’s equations, Equations (44), but now keep the polarization contribution, which yields on the left side of Equation (94) the perturbation term \( \beta \sigma P^w \). Here, \( P^w = P^w_{\text{ext}} \) is the x component of \( P^w \) in frequency domain, while a possible additional z component has been neglected. With Equation (95) and \( \beta^2 \approx \beta^2 = n_{\text{eff}}^2 c^2 / \epsilon_0 \), the perturbation term can then be written as \( \beta \sigma P^w_c \approx \Delta L H^w \), with

\[ \Delta L \approx \frac{\omega^2 n_{\text{eff}}^2}{c^2 \epsilon_0} \frac{P^w_c}{n_0^2} \]  

(101)

and Equation (94) becomes \((\hat{L} + \Delta L) H^w = \beta^2 H^w\) with \( \hat{L} = \epsilon_0 \partial_z \epsilon_\perp \partial_z + \omega^2 c^2 \epsilon_\perp \). Similarly as in Section 5.1.1, we assume that the device operates in a given transverse mode with propagation constant \( \beta \), and use that first-order perturbation theory does not affect the corresponding eigenfunction \( H^w \). Since \( \hat{L} \) is non-Hermitian, a biorthogonal basis set must be used, and the change of \( \beta^2 \) is given by \( \Delta \beta^2 = (\phi|\hat{L}|\phi)/(\phi|\phi) \). Here \( \phi = H^w \), while \( \phi \) denotes the corresponding eigenfunction of the adjoint problem \( \hat{L}^\dagger \phi(x) = \beta^2 \hat{L} \phi(x) \), with \( \hat{L}^\dagger = \epsilon_\perp \partial_z \epsilon_\parallel \partial_z + \omega^2 c^2 \epsilon_\parallel \) and \( \phi(x) \rightarrow 0 \). As can be seen by inserting Equation (95) into Equation (94), \( \beta \) simply corresponds to the conjugate complex electric field distribution of the mode \( (E^w)^* \), and in analogy to Section 5.1.1 we then obtain the field confinement factor

\[ \Gamma = \int_{\Delta_S} E^w H^w \, dx \, dy / \int_{\Delta_S} E^w \, dx \, dy \]  

(102)

Here, we have neglected a possible frequency dependence of \( n_{\text{eff}} \) and \( \Gamma \) in the last term. Obviously, our two derived Maxwell-type equations, Equations (99) and (102), have the same form as Equations (84) and (87) for TE modes, as can be seen by substituting \( H^w \rightarrow -\bar{H}^w, E^w \rightarrow \bar{E}^w, \epsilon_0 \rightarrow \epsilon_0 n_{\text{eff}}^2(\omega)/n_0^2 \omega \), \( \mu_0 \rightarrow \mu_0 n_{\text{eff}}^2(\omega)/n_0^2 \). Thus, the Maxwell-type equations in time domain can be obtained in the same way as Equation (92), yielding

\[ \partial_t E_x = -\mu_0 \frac{n_{\text{eff}}^2(\omega)}{n_0^2} \partial_y H_y \]  

(103a)

\[ \partial_t H_y = -\epsilon_0 n_0^2 \partial_x E_x - \sigma(\partial_i \partial_j \epsilon_{ij}) E_x \]  

(103b)

where the generally frequency dependent conductivity

\[ \sigma(\omega) = \epsilon_0 n_0^2 c \text{eff}(\omega) a(\omega) / n_{\text{eff}}^2(\omega) \]  

(104)

is often approximated by \( \sigma = \sigma(\omega) \). Furthermore, in the last term describing chromatic waveguide dispersion, we now have \( \text{eff}(\omega) = n_{\text{eff}}^2(\omega)/n_0^2(\omega) \). As discussed below Equation (93), certain conditions apply to \( \text{eff}(\omega) \) and \( \sigma \). In particular, they must be even functions \( f(-\omega) = f(\omega) \) to preserve the real-valued character of Equation (103). Identifying \( E_x(z, t) \) and \( H_y(z, t) \), the field strengths at the transverse position of the nanostructure, \( E_x \) can directly be used in Equation (16) or (17) to evaluate \( \partial_i \partial_j \epsilon_{ij} \). As stated above, Equation (103) has been constructed to assume the form of 1D Maxwell equations and to yield the correct propagation behavior for \( E_x \) and \( H_y \). On the other hand, the relation between \( E_x \) and \( H_y \) given by Equation (95) for \( \bar{E}^w = 0 \), is in Equation (103) for the general case of waveguide loss and dispersion only approximately fulfilled.

5.2. Slowly Varying Amplitude Approximation

As in Section 5.1, we assume a waveguiding structure which is invariant in propagation direction \( z \), and now employ the slowly varying amplitude approximation. The guided mode solutions at a given frequency \( \omega \) are characterized by the propagation constant and a z independent transverse field distribution \( F(x, y) \). Here, \( F \) is induced by the refractive index profile \( \Delta_n(x, y) \), while the polarization of the quantum systems and other nonlinear effects are assumed to act as perturbations which do not significantly affect the transverse field distribution.\(^{[181]}\)

We start from Equation (60) and introduce the slowly varying field envelopes by inserting Equation (61), where we however replace \( k_0 \) by the propagation constant of the guided mode \( \beta_0 = \beta(\omega_c) \). In the following, it is advantageous to switch to the...
spectral domain, where the slowly varying envelopes depend on the frequency variable \( \Delta_\omega = \omega - \omega_c \), corresponding to the frequency offset from \( \omega_c \). Neglecting higher-order derivatives of \( t \) and \( z \) in the spirit of the SVAA and the paraxial approximation as described in Section 4.2, and considering that time derivatives of the envelopes are replaced by multiplications with \(-i\Delta_\omega \) in frequency domain, we obtain

\[
-2i\beta_0 \partial_t \mathbf{E} + \beta_0^2 \mathbf{E} = \nabla_i^2 \mathbf{E} + \frac{\alpha^2}{c^2} \nabla_i^2 \mathbf{E} + \alpha^2 \mu_0 \mathbf{P} \tag{105}
\]

For the term \( \alpha^2 \epsilon^{-2} \nabla^2 \mathbf{E} \), we have retained the full frequency dependence of the complex refractive index \( n(x, y, \omega) \) to include chromatic dispersion, as described further below. More specifically, \( \nabla^2 = n_0^2 (1 - 2\Delta_\omega) + \sigma / (\omega \epsilon_0) \) contains the refractive index profile via \( \Delta_{n}(x, y) \) and losses via the conductivity \( \sigma \), where \( n_0, \Delta_n, \) and \( \sigma \) may be treated as frequency dependent. Assuming a guided mode solution, we can use the separation ansatz

\[
\mathbf{E}(x, t) = e \mathbf{E}(z, t) F(x, y) \tag{106}
\]

with the polarization direction of the electric field \( e \) and modal distribution \( F \). Inserting Equation (106) into Equation (105), multiplying by \( e \) and introducing the separation constant \( \beta_g \), the right side of the resulting equation becomes

\[
\left( \beta_g^2 - \frac{\alpha^2}{c^2} n_0^2 \right) F = \nabla_i^2 F \tag{107}
\]

which does not depend on the propagation coordinate \( z \). As in Section 5.1.1, \( \mathbf{P} \) is subsequently included based on first-order perturbation theory[181] Equation (107), together with the boundary condition that \( F \to 0 \) for \( x^2 + y^2 \to \infty \), constitutes an eigenvalue equation for \( F \) with complex eigenvalues \( \beta_g^2 \), featuring multiple eigensolutions which correspond to the different transverse waveguide modes. In the following, we assume that the device operates in a single transverse mode, possibly the fundamental mode. As in Section 5.1.1, we split the complex propagation constant \( \beta \) into a real and an imaginary part \( \beta = \beta_g + \text{sgn}(\beta) \alpha / 2 \) with power loss coefficient \( \alpha \), and assume that \( |\alpha| \ll |\beta| \). Including \( \mathbf{P} \) in first-order perturbation theory in analogy to Section 5.1.1 does not alter \( F \), but yields a modified propagation constant \( \beta + \Delta \beta \) with \[181\]

\[
\Delta \beta = \frac{\alpha^2}{2c^2 \beta_0} \frac{\int_{-\infty}^{\infty} \Delta_{\epsilon_i} |F|^2 dx dy}{\int_{-\infty}^{\infty} |F|^2 dx dy} \approx \frac{\alpha^2}{2c^2 \beta_0} \Gamma \Delta_{\epsilon_i} \tag{108}
\]

where \( \Delta_{\epsilon_i} = \mathbf{e} \mathbf{P}/(\epsilon_i \mathbf{E}) \) and \( \Gamma = \int_{-\infty}^{\infty} |F|^2 dx dy / \int_{-\infty}^{\infty} |F|^2 dx dy \) in agreement with Equation (88). Here, we have evaluated \( \Delta \beta \) at the carrier frequency \( \omega_c \), in accordance with the SVAA. For a realistic description of guided mode propagation, the frequency dependence of \( \beta \) itself should however be retained, giving rise to chromatic dispersion.\[181\] This effect is commonly described in terms of a Taylor series, \( \beta(\Delta \omega) = \sum_{n} (\beta_n/n! \Delta \omega) \), with \( \beta_n = [d^n \beta]_{\Delta \omega=0} \). While frequency dependent waveguide loss can be included in a similar manner by an \( \omega \) dependent coefficient \( a \), we ignore this effect since usually the spectral gain or loss profile is dominated by the contribution of the quantum systems, contained in \( \mathbf{P} \). Furthermore, assuming that \( |\Delta \beta| \ll |\beta| \) and \( \beta \approx \beta_0 \), we can approximate \( \beta_g^2 - \beta_0^2 \approx 2\beta_0 (\beta - \beta_0) + i|\beta| a + 2\beta_0 \Delta \beta \). With this result and Equation (108), the separation ansatz yields for the left-hand side of Equation (105) in time domain

\[
\frac{1}{v_g} \partial_t \mathbf{E} + \partial_z \mathbf{E} = i \sum_{n \geq 2} \frac{\beta_n}{n!} (i \partial_\omega)^n \mathbf{E} - \text{sgn}(\beta_0) \frac{a}{2} |E|^2 + i \frac{\alpha^2}{2c^2 \beta_0} \Gamma \mathbf{e} \mathbf{P} \tag{109}
\]

where \( v_g = \beta_0^{-1} \) denotes the group velocity at \( \omega_c \). The guided field solution is characterized by a linearly polarized field distribution, with the electric field pointing in direction \( e \) as reflected by the ansatz for the electric field, Equation (106).[169,181] The corresponding modes are transverse electromagnetic, that is, with transverse, perpendicular electric and magnetic fields. Notably, this approach always yields two degenerate modes, orthogonally polarized in transverse \( x \) and \( y \) directions. In reality, this applies, for example, to an ideal, cylindrically symmetric single-mode fiber, while irregularities such as random variations in the core shape already break the degeneracy. Within the assumptions of weak waveguiding, the optical power is given by the corresponding expression for the TE mode, Equation (91).

Above approach is commonly used to model coherent propagation effects in optical fibers like self-induced transparency, where the dopants, such as erbium ions, take the role of the quantum systems modeled by the Bloch equations, and the host material is, for example, glass.[189-192] Here, in addition to the refractive index profile, fiber loss, and chromatic dispersion, other effects related to the host material are also commonly considered. This, in particular, includes optical nonlinearity due to an intensity dependent refractive index of the host material, which induces an intensity dependent phase shift of the optical field and is thus referred to as self-phase modulation. This effect can be included in Equation (105) by substituting \( \beta_g^2 \) with \( \left( |n+n_\text{L}| E \right)^2 \approx n^2 + 2n_n_\text{L}|E|^2 \)[181] Treating the nonlinear component as a perturbation, we can again use Equation (108) with \( \Delta \epsilon_i = 2n_n_\text{L}|E|^2 F^2 \) and include this effect in a similar manner as discussed above. With Equations (109), (64), and (88), we finally obtain the propagation equation

\[
\frac{1}{v_g} \partial_t \mathbf{E} + \partial_z \mathbf{E} = i \sum_{n \geq 2} \frac{\beta_n}{n!} (i \partial_\omega)^n \mathbf{E} - \text{sgn}(\beta_0) \frac{a}{2} |E|^2 + i \frac{\alpha^2}{2c^2 \beta_0} \Gamma \mathbf{e} \mathbf{P} \tag{110}
\]

with the self-phase modulation coefficient

\[
\gamma = \frac{n_n \eta_\text{L}}{\beta_0 c^2} \frac{\int_{-\infty}^{\infty} |F|^2 dx dy}{\int_{-\infty}^{\infty} |F|^2 dx dy} \tag{111}
\]

We note that in Equation (111), the nonlinearity is assumed to extend over the whole fiber cross section since both the core and cladding typically consist of the same host material. The MB equations are then obtained by coupling Equation (110) to the Bloch equations in RWA, Equation (43). Here, it is practical to normalize \( F \) in Equation (106) so that \( F \approx 1 \) at the transverse...
position of the dopants acting as quantum systems; then the field in Equation (43) is directly given by \( E = e E(z, t) \).

Typically, the MB equations are stepped in time to obtain the temporal evolution of the optical field in a given geometry. For the case of unidirectional propagation along a fiber where the input at \( z = 0 \) is a given time-limited optical waveform such as a pulse, it is more practical to propagate the field in \( z \) direction. It is then convenient to introduce the retarded time variable \( \tau = t - z/v_n \), which is defined with respect to a time frame which co-propagates with the waveform. Denoting the position variable in the new coordinate system as \( \zeta = z \), we then obtain the partial derivatives \( \partial_\tau = \partial_z \). Thus, Equation (110) becomes

\[
\partial_\tau E = i \sum_{n \geq 2} \frac{\beta_n}{n!} (i \beta_n)^n E - \text{sgn}(\beta_0) \frac{a}{2} E + i y |E|^2 E + i \frac{n_{1D} a_1^2}{\epsilon_0 c \varepsilon_{\text{eff}}} \Gamma \sum_{n_{ij} > 0} d_{ij} a_{n_{ij}}
\]

where we have substituted \( \zeta \) with \( z \). For very short pulses with durations of only a few optical cycles, additional corrections may have to be included on the right side of Equation (112). In particular, this includes the self-steepening term \(-\gamma |E|^2 E\) which is a higher-order term dropped in the SVA and the Raman-induced frequency shift term \(-i \gamma_1 E \partial_z (|E|^2)\) with Raman response time \( \gamma_1 \). In Equations (110) and (112), we have assumed that \( d_{ij} \) and \( E \) are aligned in the same direction or, as is more realistic for an optical fiber, \( d_{ij} \) are effective dipole moments which average over the different orientations of the dopant ions with respect to the field. Equation (112) is solved together with the Bloch equations in RWA, Equation (43), which are expressed in the retarded time frame simply by substituting \( t \) with \( \tau \) in the density matrix elements and derivative operators. The resulting equation system is sometimes also referred to as Hirota–Maxwell–Bloch system.

5.3 Fabry–Pérot Type Resonator

For lasers, optical feedback has to be provided, which is in semiconductor lasers typically achieved by using a Fabry–Pérot type waveguide resonator. Here, the cleaved end facets provide natural reflection due to the refractive index jump between the semiconductor material and air.

5.3.1 Boundary Conditions at the End Facets

In the Fabry–Pérot type resonator, the ansatz for the optical field, Equation (61a), is extended to include a forward and a backward propagating component, with amplitudes \( F_+ \) and \( F_- \), respectively. Furthermore, assuming a guided mode solution as in Equation (106), we obtain

\[
E(z, t) = \frac{1}{2} \left[ F_+(z, t) \exp (i \beta_0 z - i \omega t) + F_-(z, t) \exp (-i \beta_0 z - i \omega t) + \text{c.c.} \right]
\]

where \( \beta_0 \) is the real part of the propagation constant at \( \omega = \omega_\text{r} \). With the (generally complex) field reflection coefficients \( r_1 \) and \( r_2 \) of the facets, assumed to be located at \( z = 0 \) and \( z = L \) where \( L \) is the resonator length, we obtain

\[
E_+(z = 0, t) = r_1 E_-(z = 0, t)
\]

\[
E_+(z = L, t) = r_2 E_-(z = L, t)
\]

where we have neglected a possible frequency dependence of \( r_1, r_2 \).

For the full Maxwell equations, a decomposition of the field into a forward and a backward propagating component is not practical. Here, reflecting boundary conditions can in principle be implemented by position dependent parameters, for example, by setting \( n_{\text{eff}} = 1 \), \( \Delta \sigma = 0 \), \( \sigma = 0 \), and \( d_{ji} = 0 \) in Equation (92b) or (103b) for \( z < 0 \) and \( z > L \) if we assume air outside of the resonator region and neglect modal effects. In this context, care has to be taken to suppress unwanted spurious reflections at the simulation domain boundaries, which can be achieved by implementing absorbing boundary conditions. However, this is not quite trivial, and various methods with different degrees of complexity have been developed. A simplified treatment, which works best for highly reflecting facets, is to use perfectly reflecting boundary conditions by setting the transverse electric field component at the facet positions to zero. The mirror loss, that is, the decay of the optical field in the cavity due to outcoupling through the mirrors, can then be considered by a distributed power loss coefficient \( a_m \), which is obtained from \( |E_\text{r} E_\text{r}|^2 = \exp(-2a_m L) \) as

\[
a_m = -\ln \left( \left| E_\text{r} E_\text{r} \right| \right)/L
\]

Using Equation (93) or (104), \( \sigma \) in Equation (92b) or (103b) can then be determined from the total power loss coefficient \( a = a_m + a_\sigma \), where \( a_\sigma = 2 \sigma_\text{eff} |\langle \beta \rangle| |\langle \beta \rangle| \) denotes the waveguide loss.

Reflection Coefficient: Using special reflective structures, such as reflection/antireflection coatings or distributed Bragg reflectors, \( r_1, r_2 \) can be custom-tailored. In the following, we focus on the highly relevant case where the bare end facets are used as reflective elements. For sufficiently large transverse waveguide dimensions, Fresnel’s formula for normal incidence can be used to estimate the field reflection coefficient at the facet as

\[
r = \frac{n_{\text{eff}} - 1}{n_{\text{eff}} + 1} = \frac{\beta - k_0}{\beta + k_0}
\]

with \( n_{\text{eff}} = \beta/k_0 \) and \( k_0 = \omega/c \). While Equation (116) is usually valid for weak waveguiding assumed in the derivation of Equations (60) and (110), modal effects can result in increased reflection at the facets. Various methods are available to compute the reflectance \( R = |r|^2 \) from the transverse mode profile.

For TE polarization, it is practical to decompose the waveguide mode, characterized by its complex propagation constant \( \beta \) and magnetic field distribution \( H_y \), which can be computed from Equation (81), into plane waves, using the Fourier transform

\[
\Phi_k(k_x) = \int_{-\infty}^{\infty} H_y(x) \exp(-ik_x x) dx
\]
Then, a generalized version of Equation (116) for tilted incidence is applied to each plane wave in order to calculate the reflection coefficient.\[198\] The reflectance $R$, that is, the ratio of the optical power reflected at the facet to the incident power, is obtained by integrating over all components, yielding

$$R = \frac{1}{2\pi} \left[ \int_{-\infty}^{\infty} |H^t_x|^2 \, dx \right]^{-1} \int_{-\infty}^{\infty} \frac{|\Phi_x|^2 \, dk_x}{k_x - k}$$

(118)

where $\kappa(\kappa_x) = \sqrt{k_x^2 - k^2}$ and the square root is chosen so that $\Im[\kappa] > 0$. From Equation (84), we see that Equation (118) can also be evaluated by replacing $H^t_x$ with $E^t_x$ in Equations (118) and (117). Making the reasonable assumption that $|\Im[\beta]| \gg |\Im[\kappa]|$, we can approximate treat the reflection coefficient $r$ as real-valued. Furthermore, assuming that the share of reflected power going into other waveguide modes is negligible,\[198\] we obtain $r = R^{1/2}$.

The case of TM polarization is somewhat more complex and can be treated based on the boundary value method.\[198\] Starting from the magnetic field distribution $H^t_x$ given by Equation (94), we first evaluate the power transmittance $T$ through the facet,\[119,198\]

$$T = \frac{2}{\pi} |\hat{P}| \left[ \int_{-k_0}^{k_0} |\epsilon_x|^{-2} |\beta^* \epsilon_x| |H^t_x|^2 \, dx \right]^{-1} \times \int_{-k_0}^{k_0} \frac{\kappa |\Phi_x|^2 |\Phi_y|^2}{\kappa |\Phi_x|^2 + \beta |\Phi_y|^2} \, dk_x$$

(119)

Here, $\Phi_x(\kappa_x)$ denotes the Fourier transform, Equation (117), of $H^t_x(x)$, and $\Phi_y(\kappa_y)$ is the Fourier transform applied to the function $\epsilon_x(x)$, with the complex relative permittivity profile of the slab waveguide structure $\epsilon_x(x)$. Again neglecting modal effects and assuming a real $r$, the reflection coefficient is then given by $r = (1 - T)^{1/2}$.

Since the field distributions and $\beta$ in Equations (118) and (119) depend on $\omega$, this also applies to the obtained reflection coefficients. Usually, this frequency dependence is neglected in the formulation of the boundary conditions, and $r$ is taken at the center frequency $\omega_c$ of the optical field.

### 5.3.2. Spatial Hole Burning

In a Fabry–Pérot resonator, the reflection at the end facets gives rise to counterpropagating waves, which produce a standing wave pattern with a periodicity corresponding to the wavelength. At the field node positions, there is no interaction of the optical field with the quantum systems. This also implies that the population inversion and resulting optical gain, as provided by the quantum systems in the active region of a semiconductor laser, do not get saturated at those positions. Thus, other modes at slightly different frequencies which have their maxima close to these unsaturated regions can also start lasing. In Figure 11, this effect is illustrated, which is referred to as (longitudinal) spatial hole burning (SHB). The resulting multimode lasing can be desired or undesired, depending on the envisaged application. For example, the broadening of the lasing spectrum is beneficial in applications such as the generation of frequency combs in QCLs, which are comb-like optical spectra used for precision metrology and sensing.\[97\] On the other hand, spatial hole burning tends to introduce optical instabilities in form of irregular variations in the mode amplitudes and phases.\[97,202\] In a similar way as just discussed for the propagation direction, SHB can also occur along the transverse directions, and has been shown to affect the spatiotemporal dynamics especially in broad-area semiconductor lasers.\[203\]

The inversion grating is smoothed out by carrier diffusion processes, and SHB can even be neglected in a first approximation if diffusion is strong enough.\[118\] Diffusion can be generically described by adding a term $\partial_i \rho_{ii, \text{diff}} = \nabla D \nabla \rho_{ii}$ to the Bloch equations, Equation (16) or (17).\[118,204\] Here, $D(x)$ is the diffusion coefficient associated with level $i$. In the following, we focus on longitudinal SHB. Furthermore, assuming constant coefficients $D_i$, the diffusion term added to the Bloch equations, Equation (16) or (17), becomes

$$[\partial_t \rho_{ii}]_{\text{diff}} = D_i \partial_z^2 \rho_{ii}$$

(120)

with zero-flux boundary conditions $\partial_z \rho_{ii} = 0$ at the resonator ends. In a two-level description of bulk semiconductors, the levels $i$ correspond to the conduction and valence bands, and the diffusion process is largely mediated by carrier–phonon and carrier–carrier scattering between the $k$ states in the bands.\[118\] In quantum wells, the levels correspond to the subbands formed by 1D carrier confinement, and the diffusion process is mediated by scattering between the $k$ states in the subbands.\[205\] In multi-quantum-dot structures, the SHB dynamics is often modeled by taking into account the carrier diffusion in the wetting layer, as well as carrier capture and escape processes to and from the quantum dots.\[206,207\] Since these processes effectively reduce the diffusion length, SHB can have a strong effect, similarly as in intersubband devices like QCLs which typically feature a very fast gain recovery dynamics.\[208\] On the other hand, the inversion grating is usually eliminated in interband bulk and quantum well lasers due to effective diffusion.\[207\]

**Slowly Varying Amplitude Approximation:** As for Equation (42), we assume that all transitions between pairs of states $i$ and $j$ with non negligible coupling to the optical field are in near-resonance, $|\omega_{ij}| \approx \omega_c$. For the corresponding off-diagonal density matrix elements, we now make the ansatz

$$\rho_{ij} = \eta^i_j(z, t) \exp \left\{ \text{sgn}(\omega_{ij}) i(\beta_i z - \omega_i t) \right\}$$

$$+ \eta^j_i(z, t) \exp \left\{ \text{sgn}(\omega_{ij}) i(-\beta_j z - \omega_j t) \right\}$$

(121)
The periodicity of the optical intensity, that is, half the wavelength. Thus, for the populations we make the ansatz

\[ \rho_{ii}(z,t) = \rho_{ii}^{0}(z,t) + \rho_{ii}^{+}(z,t) \exp(2i\beta_{0}z) + \rho_{ii}^{-}(z,t) \exp(-2i\beta_{0}z) \]

(122)

where \( \rho_{ii}^{0} = (\rho_{ii}^{0})^{*} \) correspond to the inversion grating’s amplitudes. An analogous ansatz with \( \rho_{ij}^{0} \) and \( \rho_{ij}^{\pm} \) is also chosen for off-diagonal density matrix elements which are associated with two closely aligned levels and are thus not treated in RWA, such as resonant tunneling transitions in QCLs. \([62]\) Inserting Equations (113), (114), and (122) into Equation (17) with the diffusion term Equation (120) added to Equation (17b), we obtain in a similar way as described in Section 3.5

The Bloch equations in RWA, Equation (43), are in principle analytically solvable for monochromatic excitation, corresponding to a time-constant field envelope. \([69,210]\) This is usually achieved by using the Laplace transform, which takes a time dependent function \( f(t) \) to a function \( \mathcal{L}[f](s) \) of a complex frequency variable \( s \). The main advantage is that differentiation becomes a multiplication with \( s \), that is, \( \mathcal{L}[\partial_{t} f] = s \mathcal{L}[f] - f(t = 0+) \). Restricting ourselves to a two-level system with initial conditions \( w_{0} = w(t = 0) \), and considering that the transform is linear and \( \mathcal{L}[1] = s^{-1} \), Equation (73) becomes in Laplace domain

\[ \mathcal{L}[\eta_{21}] = s^{-1}[-i\mathcal{L}[w]2\Omega_{g} + \eta_{01}^{0}] \]  

(125a)

\[ \mathcal{L}[\eta_{12}] = s^{-1}[i\mathcal{L}[w]2\Omega_{g} + (\eta_{01}^{0})^{*}] \]  

(125b)

\[ \mathcal{L}[w] = \frac{2\gamma_{1} + w \gamma_{2} + \gamma_{s} \gamma_{s}}{s \gamma_{s} \gamma_{s} + (s + \gamma_{2})(s + \gamma_{2}) + \eta_{21}^{0} \Omega_{g}^{2}} \]  

(125c)

with \( s_{\pm} = (s + \gamma_{s} \pm \Delta \Omega_{g} / 2) \) and \( s_{0} = \mathcal{L}[\eta_{21}^{0} \Omega_{g}] \). Here, the off-diagonal matrix elements have already been eliminated in Equation (125c) by inserting Equations (125a) and (125b). Back-transformation of Equation (125c) is achieved by performing a partial fraction decomposition, which results in a sum of simpler fractions with known inverse Laplace transforms. This requires finding the poles of the rational function in Equation (125c), given by \( s = 0 \) and the roots of the cubic function of \( s \) in the square brackets of the denominator, for which closed analytical expressions are readily available. The solution for \( f(t) = w(t) \) and \( f(t) = \eta_{21}(t) \) is of the form \([49]\)

\[ f(t) = A + B \exp(-at) + [C \cos(\omega t) + D \sin(\omega t)] \exp(-bt) \]

where the decay constants \( a \) and \( b \) and the oscillation frequency \( \omega \) are the same for \( w \) and \( \eta_{21} \), but the coefficients \( A, B, C, D \) are different and also depend on the initial conditions.

Rabi Oscillations: In the following, we consider the case of dissipationless light–matter interaction, that is, \( \gamma_{1} = \gamma_{2} = 0 \). Then, Equation (125c) becomes

\[ \mathcal{L}[w] = \frac{2\gamma_{1} + w \gamma_{2} + \gamma_{s} \gamma_{s}}{s \gamma_{s} \gamma_{s} + (s + \gamma_{2})(s - \gamma_{2})} \]

(126)
where $\Omega_g = (\Delta^2 + |\Omega|^2)^{1/2}$ denotes the generalized Rabi frequency for detuned excitation, and $A = \Omega_g^{-2}(2\Delta\Re\{n_{21}^0\Omega^0\}) + \Delta^2w_0$. Inverse Laplace transformation of Equation (126) yields

$$w(t) = A + (w_0 - A) \cos(\Omega_g t) + 2\Omega_g^{-1}3\{n_{21}^0\Omega^0\} \sin(\Omega_g t)$$ (127)

As can be seen from Equation (127), a monochromatic, nearresonant light field interacting with an ideal, dissipationless two-level system causes Rabi flopping, that is, an oscillation of the population between states 1 and 2 with frequency $\Omega_g$, as predicted by Rabi for the analogous case of a two-level system in a rotating magnetic field.[14] In Figure 12, $w(t)$ is shown for the initial conditions $w_0 = -1, n_{21}^0 = 0$, and different detunings. As can be seen, complete population inversion with $w = 1$ is achieved only for resonant excitation.

Due to the presence of dissipation, above presented analytical treatment of Rabi flopping can rarely be directly used for the description of optoelectronic device operation. However, under favorable conditions, signatures of Rabi oscillations have been observed in nanostructured optoelectronic systems and devices.[15,17] QCLs,[18] single quantum dots,[19,20] and nanowire lasers[6] at cryogenic temperatures, as well as quantum dots[21-23] and quantum dash[24] amplifiers at room temperature. Besides the usually strong influence of dissipation, effects beyond the two-level dynamics and inherent restrictions of models based on macroscopic Maxwell–Bloch equations, the applicability of Equation (126) is also limited by the validity range of the RWA. In particular, for very strong optical excitation where the Rabi frequency approaches the optical resonance frequency, effects beyond the RWA have been observed in bulk and nanostructured semiconductors.[105,211-213]

**Steady-State Solution:** In the following, we consider the steady-state behavior for a dissipative two-level system under monochromatic optical excitation, that is, for a field at frequency $\omega$, with constant amplitude. In the presence of dissipation, the coherent transients associated with above discussed Rabi oscillation, Equation (127), decay, and the system approaches the steady state for $t \to \infty$. The steady-state solution can be obtained by setting $\dot{\eta}_i = 0$ in Equation (73). Alternatively, we can apply the final value theorem to Equation (125), stating that if $\lim_{t \to \infty} f(t)$ exists, it is identical to $\lim_{s \to 0} sL(f)$. Introducing the relaxation times $T_{r1,2} = \gamma_{r1,2}^{-1}$, we then obtain

$$\eta_{21} = \frac{1}{2} \frac{\Omega T_2(\Delta T_2 - i)w_{eq}}{1 + \Delta^2 T_2^2 + T_1 T_2 |\Omega|^2}$$ (128a)

$$w = \frac{(1 + \Delta^2 T_2^2)w_{eq}}{1 + \Delta^2 T_2^2 + T_1 T_2 |\Omega|^2}$$ (128b)

From Equation (128), an expression for the relative permittivity $\varepsilon_r$ and susceptibility $\chi_r = \varepsilon_r - 1$ due to the quantum systems can be derived. Setting the classical expression for the complex polarization amplitude $P = \varepsilon_0 \chi E$ equal to Equation (75), we obtain with Equation (128a), $\Omega = \hbar^{-1}d_{21}E$ and Equation (89) the frequency and intensity dependent susceptibility[15,17]

$$\chi = \frac{\varepsilon_0 n_{21}|d_{21}|^2 T_2}{\omega^2} \frac{(\Delta T_2 - i)w_{eq}}{1 + \Delta^2 T_2^2 + I/I_s}$$ (129)

with the saturation intensity at zero detuning

$$I_s = \frac{\hbar^2 \varepsilon_0 n_{21} c}{2T_1 T_2 |d_{21}|^2}$$ (130)

For arbitrary detuning, the saturation intensity is then given by $I_s(1 + \Delta^2 T_2^2)^{1/2}$ that is, nonresonant fields interact less strongly with the two-level system, and thus saturation occurs for higher intensities. As in Section 5.2, it is here assumed that $d_{21}$ and $E$ are aligned in the same direction, or that $d_{21}$ is an effective value averaged over the different orientations of, for example, dopant ions in an optical fiber.

In Figure 13, the real and imaginary parts of $\chi$ are shown as a function of detuning from the optical resonance frequency for various optical intensities. $\Re\{\chi\}$, which contains chromatic
dispersion, changes sign at the resonance frequency. \( \Im(\chi) \) describes gain for \( w_{eq} > 0 \), that is, positive population inversion, and loss for \( w_{eq} < 0 \), where the frequency dependence is given by a Lorentzian profile with the full width at half-maximum (FWHM) bandwidth \( 2\gamma_0(1 + I/I_L)^{1/2} \). For increased intensities, the profile thus gets broadened which is known as power broadening, and also the peak value at resonance frequency is reduced by a factor of \( 1 + I/I_L \), which corresponds to gain saturation for \( w_{eq} > 0 \) and saturable absorption for \( w_{eq} < 0 \).

In the following, we investigate optical power amplification or absorption by two-level systems. For TE modes or generally in the limit of weak waveguiding, the power is given by Equation (91). Multiplying Equation (110) from left with \( \bar{E}^* \) and adding the complex conjugate, we obtain with Equations (128a) and (91) and \( \beta_0 = \omega_0 n_{eff} / c \)

\[
\partial_z P = -a P + g P
\]

where \( a \) is the waveguide loss coefficient, and the two-level power gain coefficient is given by

\[
g = \alpha \frac{w_{eq}}{1 + \Delta^2 T_2^2 + P/P_0}
\]

with

\[
\alpha = \Gamma \frac{\alpha_{0\ell} |d_{12}|^2 T_2}{\varepsilon_0 c \hbar n_{eff}}
\]

and the saturation power at zero detuning \( P_s = A_0 \ell L \). With the help of the Lambert W function, defined by \( x = W(x) \exp[W(x)] \), we can write the solution of Equations (131) and (132) for zero waveguide loss, \( a = 0 \), as \( P(z) = P_0 G(z) \) with the power gain factor

\[
G(z) = \frac{P_0'}{P_0} W\left(\frac{P_0}{P_0'}\right) \exp\left(\frac{\alpha w_{eq}}{1 + \Delta^2 T_2^2} z\right)
\]

where \( P_0 = P(z = 0) \) and \( P_0' = (1 + \Delta^2 T_2^2) P_s \). With Equation (134), the steady-state field solution of Equation (110) can then for \( a = 0 \) be written as

\[
\bar{E}(z) = \bar{E}(z = 0) |G(z)|^{1/(1 + \Delta T_2^2)^2}
\]

and the density matrix elements are with \( \Omega = \hbar^{-1} d_{12} \bar{E} \) given by Equation (128). In the exponent of Equation (135), \( \alpha_{d1} = -\Delta T_2 \) corresponds to the Hooke or linewidth enhancement factor, which relates phase changes to changes in the optical gain.

In Figure 14, the optical power gain and phase shift of the electric field as a function of propagation distance for different values of initial power \( P_0 \) for \( w_{eq} > 0 \), that is, amplification. In the small signal limit, \( P < P'_0 \), the typical exponential increase in power is observed. This can also be seen from Equation (134), which yields with \( W(x) \approx x \) for \( x \ll 1 \) the usual exponential amplification for \( G > 1 \) or loss for \( G < 1 \) characteristics. In the saturation regime, the power increases only linearly. Physically, this is a consequence of the fact that the growth in optical power is ultimately limited by the supplied pump power.

The expressions Equations (129) and (132) for the susceptibility \( \chi \) and optical gain \( g \) are widely used to model the optical properties of homogeneously broadened atomic\(^{[157,170]} \) and nanostructured\(^{[213,216]} \) optical media. In particular for interband transitions in bulk semiconductor and quantum well media, the electron wavevector must be explicitly considered, along with additional corrections due to Coulomb interactions.\(^{[65,67]} \) Above derivation of an expression for the susceptibility from the Bloch equations can be extended to more than two levels, which is, for example, relevant for the investigation of slow light propagation. This is usually achieved based on electromagnetically induced transparency (EIT), where a control laser beam induces a narrow transparency window with an extremely low group velocity in the absorption spectrum of a suitable medium.\(^{[217–219]} \) EIT requires a three-level configuration, and expressions for the susceptibility have been derived in a similar way as above.\(^{[35,219]} \) A reduction of the group velocity to subsonic speeds, as well as complete halting of light, has been demonstrated in an ultracold atomic vapor.\(^{[32–34]} \) Possible applications include optical buffers,\(^{[38]} \) imaging,\(^{[36,37]} \) and quantum memory.\(^{[38]} \) In view of a future commercialization of these technologies, a compact solid-state-based implementation is desirable, and slow light propagation as well as light trapping has meanwhile been demonstrated in doped crystals.\(^{[35,46]} \) The realization of slow light in suitably engineered semiconductor structures is especially attractive. Here, the exploitation of tunneling induced transparency is highly promising, which differs from EIT in that it does not require an optical control field, but utilizes strong tunneling coupling between a pair of states. For this case, the susceptibility has been analytically derived for quantum dot and intersubband quantum well systems.\(^{[41–43]} \) Furthermore, nonlinear optical mixing effects which involve optical field contributions at two or more frequencies, and often rely on more than two energy levels, are exploited in many semiconductor-based applications, requiring a description by higher-order susceptibilities.\(^{[228–227]} \) The corresponding expressions can, for example, be obtained from the Bloch equations by employing time-dependent perturbation theory.\(^{[228,229]} \)
6.1.2. Self-Induced Transparency

In addition to above presented steady-state solution to the Maxwell–Bloch equations, dynamic solutions are also available for some special cases. An important example is self-induced transparency (SIT), where a special optical pulse solution exists which can propagate through the two-level medium without being attenuated or disturbed. This effect was theoretically predicted, and first experimentally demonstrated in ruby, by McCall and Hahn.\textsuperscript{[24,25]} SIT is based on coherent interaction with the medium, which requires that the pulse duration must be much shorter than the relaxation processes described by $\gamma_1$ and $\gamma_2$, and thus we can set $\gamma_1 = \gamma_2 = 0$. Furthermore, we assume that the field envelope $\Omega = h^{-1}d_{12}F$ is real-valued, and initially restrict ourselves to resonant excitation, that is, $\Delta = 0$. Then, the solution of Equation (74) for the initial condition $s_1(z, -\infty) = s_2(z, -\infty) = 0$, $w(z, -\infty) = -1$ can be written as $s_1 = 0$, $s_2 = -\sin \vartheta$, and $w = -\cos \vartheta$ with $\vartheta(z, t) = \int_{-\infty}^{t} \Omega(z, t')dt'$, as can easily be verified by re-insertion of the solution into Equation (74). This analysis can be extended to incorporate inhomogeneous broadening in media consisting of quantum systems with slightly different resonance frequencies.\textsuperscript{[49,109]} Assuming that nonresonant systems with $\Delta \neq 0$ essentially respond in the same way to $\Omega$ as the resonant ones, apart from a change in amplitude, we can make the factorization ansatz $s_{2,\Delta}(z, t) = F(\Delta) s(z, t)$, which again yields closed analytical solutions to Equation (74).

$$s_{2,\Delta}(z, t) = -F(\Delta) \sin \vartheta(z, t)$$  \hspace{1cm} (136)

$$w_{\Delta}(z, t) = -F(\Delta) \cos \vartheta(z, t) - 1$$  \hspace{1cm} (137)

Taking the second derivative of Equation (74b) for $\Delta \neq 0$ and inserting Equations (74a), (136), and (137) yields

$$\partial_t^2 \vartheta = \frac{\Delta^2 F(\Delta)}{1 - F(\Delta)} \sin \vartheta : = T^{-2} \sin \vartheta$$  \hspace{1cm} (138)

Since the electric field envelope, and hence also $\vartheta$, is $\Delta$ independent, this must also apply to $\Delta^2 F(\Delta)[1 - F(\Delta)]$ which we have thus set equal to a constant $T^{-2}$ in Equation (138). This yields a Lorentzian dependence $F = 1/(1 + T^2 \Delta^2)$. Equation (138) corresponds to the pendulum problem, where the solutions are given by elliptic functions. Here, we require $\Omega = \vartheta, \Omega = 0$ and thus $\partial_t \vartheta = \partial_t^2 \vartheta = 0$ at $t = \pm \infty$, yielding the unique solution $\vartheta = 4 \arctan[\exp(t - t_0)/T]$. Introducing $b_0 = z/v$ with the pulse propagation velocity $v$, we thus obtain

$$\Omega(z, t) = 2T^{-1} \text{sech}(\tau / T)$$  \hspace{1cm} (139)

with the retarded time variable $\tau = t - z/v$.

In the optical propagation equation, inhomogeneous broadening can approximately be included by substituting $s_1 - is_2$ with $\int_{-\infty}^{\infty} g(\Delta) d\Delta$ in the polarization, Equation (75), where $g(\Delta)$ with $\int_{-\infty}^{\infty} g(\Delta) d\Delta = 1$ gives the distribution of quantum systems as a function of the detuning $\Delta$ from $\omega_0$. Here, a possible dependence of the dipole matrix element on $\Delta$ has been neglected. Using $s_{2,\Delta} = F(\Delta) s_2$ and above result for $F(\Delta)$, we obtain $s_{2,\Delta} = s_{2,\Delta}$, and with Equation (74a) we see that then

$$s_{1,\Delta} = -s_{1,\Delta} \text{ for } \Omega = \vartheta = 0.$$  \hspace{1cm} (140)

Often $g(\Delta)$ is an even function as further discussed in Section 8.2, and then the contribution of $s_{1,\Delta}$ cancels out. Under this assumption, Equation (110) becomes without dispersion ($\beta_0 = 0$ for $n \geq 2$), loss ($\alpha = 0$) and self-phase modulation ($\gamma = 0$)

$$\partial_t \Omega + \vartheta \partial_t \Omega = 2^{-1} \alpha \gamma_2 \vartheta s_2 \int_{-\infty}^{\infty} g(\Delta) F(\Delta) d\Delta$$  \hspace{1cm} (141)

where $\alpha$ is given by Equation (133). Inserting Equations (139) and (136) into Equation (140) yields the pulse propagation velocity

$$v = \frac{2}{2 + \alpha \gamma_2 \vartheta T^2 \int_{-\infty}^{\infty} g(\Delta)[1 + T^2 \Delta^2]^{-1} d\Delta}$$  \hspace{1cm} (141)

In Figure 15, the pulse shape, inversion $w$, and the imaginary part of the off-diagonal matrix element $\Im{\Omega_{12}} = -s_{2}/2$ is shown. Notably, for $w_{\text{eq}} < 0$ when the two-level medium normally absorbs light (see Equation (132)), the optical energy absorbed during the first half of the SIT pulse and stored in the inversion, is re-emitted during the second half, which delays the pulse so that $v$ is smaller than the group velocity $v_g$ without the coherent interaction as can be seen from Equation (141), but does not change its shape or amplitude. This is accompanied by a Rabi flop of the population inversion from $w = -1$ to $w = 1$ and back again.

Generally, based on the area theorem, it was found that for coherent propagation, the pulse area $a \equiv \int \Omega dt$, evolves toward the closest even multiple of $\pi$ ($\Theta = 0, 2\pi, 4\pi, \ldots$) for absorbing media ($w_{\text{eq}} < 0$), and to the closest odd multiple of $\pi$ for gain media ($w_{\text{eq}} > 0$).\textsuperscript{[20]} Importantly, the area theorem only makes a statement about $\Theta$, but does not indicate if the pulse envelope changes. As discussed above, the SIT pulse Equation (139), which has a pulse area $\Theta = 2\pi$, is the only finite energy solution of Equation (138) where the pulse envelope is preserved. However, analytical solutions of the MB equations with changing pulse shapes can also be obtained for other cases of coherent propagation.\textsuperscript{[219,231]}

With regards to novel practical applications, SIT is, for example, a highly interesting candidate for the generation of ultrashort optical pulses in various types of lasers with sufficiently long coherence times, such as quantum dot and quantum cascade lasers.\textsuperscript{[27–31,121,232,233]} This SIT (or coherent) mode-locking approach requires a laser design with one or multiple gain and absorber regions, where an SIT soliton with a pulse area of

---

**Figure 15.** Self-induced transparency soliton. Shown are a) the normalized electromagnetic field and b) inversion $w$ and imaginary part of the off-diagonal matrix element $\Omega_{12}$, where $\Im{\Omega_{12}} = 0$. 

---

Mathematical equations and expressions used in the text:

1. $s_{1,\Delta} = -s_{1,\Delta}$ \text{ for } $\Omega = \vartheta = 0$.
2. $\partial_t \Omega + \vartheta \partial_t \Omega = 2^{-1} \alpha \gamma_2 \vartheta s_2 \int_{-\infty}^{\infty} g(\Delta) F(\Delta) d\Delta$.
3. $v = \frac{2}{2 + \alpha \gamma_2 \vartheta T^2 \int_{-\infty}^{\infty} g(\Delta)[1 + T^2 \Delta^2]^{-1} d\Delta}$.
\[ d_{12} \int E(t) dt / \hbar = 2\pi \]
is approximately realized in the absorber sections. In order to obtain a stable pulse area of \( \pi \) in the gain regions, they are engineered to have half the dipole moment \( d_{12} \) of the absorber sections. Instead of sequential gain and absorber regions, another option is to stack the gain and loss regions in transverse direction, that is, perpendicular to the propagation axis. This approach is, for example, compatible with the manufacturing process of QCLs, and an analytical solution has been derived for the steady-state pulse solution.\(^{[30]}\) Despite its great promise, SIT mode-locking has not been experimentally demonstrated to date.

### 6.2. Full-Wave Bloch Equations

Without employing the RWA, the Bloch equations (17) are solvable only for very special conditions. In particular, for \( |\Delta M| = 1 \) transitions in hydrogen-like atoms where the dipole matrix element is given by \( d = 2^{-1/2}|d(e_1 - ie_1)| \), excitation with circularly polarized light where \( E_x = E(t) \cos(\omega t) \) and \( E_y = E(t) \sin(\omega t) \) leads to \( dE(t) = 2^{-1/2}|d| E(t) \exp(-i\omega t) \).\(^{[14],[49]}\) Furthermore, using Equation (42) to substitute the off-diagonal density matrix elements in Equation (17), the resulting equation formally corresponds to the RWA Bloch equation, with the analytical solutions discussed in Section 6.1. Closed analytical solutions are not available for the relatively simple, but very important case of monochromatic excitation with a linearly polarized wave. Some approximate corrections have been derived, such as the Bloch–Siegert shift describing the change in the system’s resonance frequency for strong driving,\(^{[155]}\) and the Mollow triplet which refers to the emergence of satellite peaks in the spectrum of resonantly excited systems.\(^{[234]}\) Interestingly, the full Bloch equations can be solved analytically if the linearly polarized electric field has the form of an \( N \)-soliton. This is also true for the so-called reduced MB equations, which combine the full-wave Bloch equations with a first-order unidirectional optical propagation equation.\(^{[235,236]}\)

### 7. Numerical Schemes

As discussed in Section 6, the full-wave MB equations have known analytical solutions only for very special cases, and also in the RWA/SVAA approximation, no general analytical solution exists. Therefore computer simulations are in general necessary. From a practical point of view, the numerical scheme should be stable, accurate, and efficient, and a naive discretization will often fail. The goal of this section is to introduce well-established approaches which are straightforward to implement, and give a critical discussion of their properties. Furthermore, an overview of recent developments in the field will be given. Since the RWA/SVAA problem and the full MB equations are not of the same mathematical form, their numerical implementation has to be treated separately.

Several software projects have been published that are able to solve the Maxwell–Bloch equations. For example, the Freewtm project\(^{[257]}\) is an open-source MATLAB code that simulates the dynamics of semiconductor lasers using the 1D MB equations in rotating wave approximation. The Electromagnetic Template Library (EMTL) is a free C++ library with Message Passing Interface (MPI) support,\(^{[238]}\) which has, for example, been used to model quantum emitters with the full-wave MB equations in two dimensions.\(^{[239]}\) Another solver library for the full-wave MB equations is the open-source MEEP project,\(^{[240]}\) using a similar representation of the Bloch equations as given in Equation (72). The mbsolve project\(^{[241]}\) solves the full-wave MB equations using different parallel acceleration techniques and features an open-source codebase. Finally, a commercial MB solver has been announced.\(^{[242]}\)

#### 7.1. Rotating Wave/Slowly Varying Amplitude Approximation

##### 7.1.1. Finite Difference Discretization of the 1D Propagation Equation

In the following, the numerical solution of the 1D optical propagation equation in the SVAA is discussed. Neglecting chromatic dispersion, that is, setting \( \beta_n = 0 \) for \( n \geq 2 \), we write Equation (124) in the form

\[
\partial_t E^\pm = \mp v_g \partial_z E^\pm + f^\pm(z,t) - \ell E^\pm \tag{142}
\]

An obvious choice is to use a finite difference discretization approach where a spatiotemporal discretization of \( E^\pm \) onto an equidistant grid with \( z_n = m \Delta z, t_n = n \Delta t \) is imposed. In the following, \( E^\pm_{m,n} \) and \( f^\pm_{m,n} \) denote the numerical solution of \( E^\pm \) and \( f^\pm \) on the grid. The starting point is a Taylor series expansion of \( E^\pm(z_n, t_{n+1}) \) around the point \( (z_n, t_n) \), yielding up to second order

\[
E^\pm_{m,n+1} = E^\pm_{m,n} + \ell \frac{\partial^2}{\partial z^2} E^\pm_{m,n} + \Delta z^2 \frac{\partial}{\partial z} f^\pm_{m,n} \tag{143}
\]

Then, \( \partial_z E^\pm_{m,n} \) and \( \partial^2 z E^\pm_{m,n} \) are replaced by space derivatives. Differentiating Equation (142) with respect to \( z \), multiplying the result by \( \mp v_g \) and adding it to the time derivative of Equation (142) yields

\[
\mp v_g \partial_z E^\pm_{m,n} + f^\pm_{m,n} + \ell E^\pm_{m,n} \tag{144}
\]

For finite difference discretization, there are different possibilities such as the well known and widely used second-order Lax–Wendroff method,\(^{[243]}\) or the Risken–Nummedal finite differences (RNFD) scheme which was specifically developed in the context of MB simulations.\(^{[244]}\) In both cases, \( \partial^2 z E^\pm_{m,n} \) is approximated by the standard finite difference approximation \( E_{m+1,n} - 2E_{m,n} + E_{m-1,n} / \Delta z^2 \). Here, we will treat in detail the RNFD scheme, since it has some advantageous properties as discussed further below. The main difference as compared to the Lax–Wendroff method is that rather than employing centered differences, depending on the propagation direction backward/foward finite differences are used, with \( \partial_z E^\pm_{m,n} \approx \ldots \)
Numerical Properties of the RNFD Scheme: For a numerical scheme to be useful, an important requirement is that round-off and truncation errors do not get amplified during the computation, since this will eventually lead to numerical instability. The stability of finite difference discretization schemes can be investigated based on a von Neumann stability analysis. It turns out that the RNFD scheme is stable for $\ell \geq 0$, which is also true for the Lax–Wendroff method for a sufficiently small Courant number $\nu_{\ell} \Delta_t / \Delta_x$. On the other hand, for positive linear gain, that is, $\ell < 0$, we obtain unconditionally unstable behavior for both schemes. Furthermore, like the Lax–Wendroff method, the RNFD scheme is second-order accurate in space and time. This guarantees that the numerical scheme converges to the original partial differential equation as the grid spacing approaches zero, with a convergence order of two. However, this does not yet guarantee that the numerical solution for finite grid spacing has a physically meaningful behavior, for example, satisfies certain physical conservation laws. Thus, additional conditions might be desirable for a finite difference discretization of Equation (142), which has the form of an inhomogeneous scalar convection equation and thus allows us to draw from related work. Specifically, it has been established that second- and higher-order linear finite difference schemes tend to introduce artificial numerical dispersion, yielding phase errors and numerical oscillations near extrema or discontinuities of the solution. The numerical solution is less prone to phase errors for monotonicity preserving schemes, which guarantee that for every nondecreasing (nonincreasing) initial condition $E_{m,n}^{\pm,0}$, the numerical solution at all later instants $n > 0$ is also nondecreasing (nonincreasing). A sufficient condition for the RNFD scheme to be monotonicity preserving for the homogeneous propagation equation, that is, Equation (142) with a vanishing source term $f^\pm(z, t) \equiv 0$, can be easily derived. Formulating Equation (145) for $E_{m+1,n+1}^{\pm}$ and subtracting the resulting expression from Equation (145), we arrive at

$$E_{m+1,n+1}^{\pm} - E_{m,n+1}^{\pm} = (1 - \ell \Delta_t)(E_{m+1,n}^{\pm} - E_{m,n}^{\pm}) + \frac{\Delta_t^2}{2} \ell^2 (E_{m+1,n}^{\pm} - E_{m,n}^{\pm})$$

which yields $\Delta_t \leq 1/|\ell|$ as sufficient condition for monotonicity preservation in the stability regime $\ell \geq 0$. This is a unique feature for a second-order finite difference propagation scheme which is directly related to the choice of time step $\Delta_t = \Delta_x / \nu_{\ell}$. Also, this constitutes an important advantage of the RNFD scheme over the Lax–Wendroff method, which does not have this property in numerically stable regions, as can be shown in a similar way as above or directly from Godunov’s order barrier theorem.

In Figure 16, the Lax–Wendroff and the RNFD scheme are compared for lossless propagation of an initially rectangular pulse without interaction with a quantum system. For the Lax–Wendroff scheme, spurious oscillatory features arise in the vicinity of the field discontinuities, which are absent in the RNFD scheme due to its monotonicity preserving nature.

7.1.2. Density Matrix Equations

The numerical scheme for the optical propagation equation has to be coupled to a time-propagation scheme for the Bloch equations, Equation (43). These constitute an ordinary differential equation (ODE) system describing the temporal evolution of the density matrix, which has to be solved for each spatial grid point. In principle, most standard methods should do the job although they will differ in numerical stability, accuracy, and efficiency, and well-established schemes such as Runge–Kutta and Adams–Bashforth have successfully been used. Most research on the suitability of different numerical schemes in literature has focused on the full-wave Bloch equations, as detailed in Section 7.2. Since they are identical in structure to the RWA Bloch equations (compare, e.g., Equations (67a) and (68) to Equation (73)), the obtained insights should in principle also be valid for the RWA Bloch equations. The Runge–Kutta method is further described in Section 7.2.4 in the context of full-wave Bloch equations. Here, we exemplarily discuss the explicit Adams–Bashforth scheme as an especially straightforward to implement and numerically highly efficient method. The RNFD scheme for the MB equations, Equation (145), is strongly coupled, that is, requires an evaluation of the density matrix and the electric field at the same time value. The $k$-step Adams–Bashforth method for the solution of an ODE system is given by

$$\rho^{n+1} = \rho^n + \Delta_t \sum_{m=0}^{k-1} c_m f^{n-m}(\rho^{n-m})$$

(146)
Here, \( n \) corresponds to the time \( t_n = n \Delta t \), \( \Delta t \) is the time step size, and \( F(\hat{\phi}) = L(\hat{\phi}) + D(\hat{\phi}) \) represents the right hand side of the Lindblad equation (3), and specifically in our case of the RWA Bloch equations, Equation (43). Furthermore, the \( c_{\omega k} \) are suitably chosen coefficients\(^{[251]} \) so that maximal accuracy is reached in the approximation. A \( k \)-step Adams–Bashforth method has a global numerical error on the order of \( O(\Delta t^k) \).\(^{[252]} \) In this context, it must be considered that the overall numerical accuracy cannot be arbitrarily improved by choosing a high value of \( k \), since it is also limited by the numerical discretization of the optical propagation equation, for example, based on the RNFD method. As discussed in Section 4.3, the Bloch equations are initialized by the starting values of the density matrix elements at a given time, while the Adams–Bashforth method would require \( k \) initial values as can be seen from Equation (146). This problem can, for example, be solved by doing the first \( k - 1 \) time steps with a different numerical scheme such as the Runge–Kutta method, or by initializing the simulations with two-step Adams–Bashforth on a finer grid. In simulations of laser operation which are typically started from noise,\(^{[173]} \) the exact choice of initial conditions is not critical and thus the initialization steps required by Adams–Bashforth do not pose a problem. The main advantage is the reduced numerical load as compared to the Runge–Kutta method (see Section 7.2.4), which however requires initialization only at a single time point.

7.1.3. Generalizations and Alternative Methods

In Section 7.1.1, 1D propagation has been assumed, neglecting the transverse coordinates in the SVAA propagation equation, Equation (62). In reality, the field dependence, and thus also the temporal evolution of the quantum systems, is varying along the \( x \) and \( y \) coordinates, which must be explicitly considered for an inclusion of diffraction and other effects.\(^{[249,254]} \) As long as no transverse boundary conditions or material dependencies have to be considered, that is, \( \Delta_x \) and \( \sigma \) in Equation (62) are constant, the most straightforward approach is to Fourier-transform Equation (62) with respect to \( x \) and \( y \) before the time propagation step is carried out.\(^{[249]} \) The resulting equation then depends on \( z \), \( t \) and the spatial Fourier frequencies \( k_x \) and \( k_y \), converting the derivative operator \( \nabla \) into a multiplication with \( -(k_x^2 + k_y^2) \). Thus a 1D propagation method can be used, such as the one discussed in Section 7.1.1. Since this procedure requires a Fourier transform before and an inverse transform after each propagation step, the numerically efficient fast Fourier transform method is usually employed.

As discussed in the context of Equation (112), for the modeling of unidirectional fiber or beam propagation, often the initial field at \( z = 0 \) is given, and the solution at a certain distance \( z = L \) is required. Then it is more practical to propagate the field in \( z \) direction rather than in time, and to introduce the retarded time variable \( \tau = t - z/v \), which simplifies the propagation operator \( \left( v_y^{-1} \partial_z + \partial_t \right) \) to \( \partial_\tau \). In the absence of other time derivatives, for example, due to chromatic dispersion, this effectively reduces the propagation equation to an ODE. The solution is then marched in \( z \) direction in dependence of \( \tau \) (and \( k_{x,y} \) if applicable), and the density matrix is updated after every propagation step.\(^{[249,250]} \) The propagation along \( z \) can be performed with a conventional ODE scheme where, for example, the Adams–Moulton method (with the trapezoidal rule as a widely used special case) or Adams–Bashforth method, Equation (146), have been employed, in both cases combined with fourth-order Runge–Kutta for the Bloch equations.\(^{[249,250]} \) In the more general case where time derivatives have to be considered in Equation (112), for example, to incorporate chromatic dispersion, these can be handled in Fourier domain, similarly as for the \( x \) and \( y \) derivatives discussed in the previous paragraph. One option is to process all terms in Fourier domain,\(^{[255]} \) which however complicates the treatment of expressions which are nonlinear in the field, such as the self-phase modulation term in Equation (112). Another strategy might be to couple the Bloch equations to the split-step Fourier method, which treats only the terms containing time derivatives in Fourier domain, and the others in time domain.\(^{[183]} \)

7.2. Full-Wave Simulation

While the RWA significantly reduces the computational workload, care must be taken in cases where its basic assumptions are not fulfilled. For example, the RWA assumes that the electric field intensity is small and the field spectrum narrow. However, in a scenario where ultrashort pulse generation is simulated (e.g., mode-locking operation in quantum cascade lasers), the electric field features high peak intensity and a broad spectrum. In such cases, the full electromagnetic wave might have to be considered in the simulation, and a suitable numerical scheme has to be used. In the following, we describe the methods for the Maxwell and full-wave Bloch equations, Equations (44) and (17), which are most widely used in related literature, and address the coupling between the updates of the electric field and the density matrix. Finally, we assess the advantages and drawbacks of the different methods.

7.2.1. Numerical Schemes for Maxwell’s Equations

Out of the many numerical methods that solve Maxwell’s Equations, mainly two—namely the finite-difference time-domain (FDTD) and the pseudo-spectral time-domain (PSTD) method—are used in the context of Maxwell–Bloch equations. The FDTD method is one of the standard methods for Maxwell’s equations,\(^{[54]} \) and is widely used in combination with the optical Bloch equations.\(^{[53–60,102,103,175,236,237]} \) Here, the derivatives with respect to time and space are approximated using central differences. Hence, the method has second-order accuracy. In order to facilitate the calculation of the central differences, the Yee grid is used where the discretization points are staggered by half of the respective step size.\(^{[238]} \) Figure 17 depicts an example of a Yee grid in one spatial dimension. The main advantage of the FDTD scheme is its simplicity. The implementation of the method as well as boundary conditions or sources is straightforward.\(^{[52]} \) Additionally, it can be executed efficiently in parallel, although the naive implementation will not yield the maximum performance and a more advanced approach must be used.\(^{[259,260]} \) The major drawback is the introduced numerical dispersion which can only be avoided by using very fine
discretization sizes. Otherwise, artifacts in the simulation results could be the consequence. In the context of MB simulations, different values (and value ranges) for the maximal spatial discretization size $\Delta_z$ have been found adequate for the FDTD scheme. Namely, $\lambda/20 \leq \lambda/100$, $\lambda/50$, $\lambda/100$, and $\lambda/200$ have been used, where $\lambda$ represents the smallest occurring wavelength. The maximum time step $\Delta t$ is, similarly as in Section 7.1.1, determined by the Courant number, which leads for the FDTD scheme to the condition $v\Delta t \leq \Delta z$ (or $v\Delta t \leq (\Delta x^2 + \Delta y^2 + \Delta z^2)^{-1/2}$ for three spatial dimensions). Here, the velocity is obtained from the parameters in Equation (44) as $v = (\mu_0\varepsilon_0\epsilon)^{-1/2}$. In related literature, choosing $v\Delta t = \Delta z/2$ was found to be adequate.\(^{102,261}\)

To reduce the numerical burden, different approaches using the pseudo-spectral time-domain method\(^{262}\) have been presented.\(^{154,263}\) This method calculates the spatial derivatives using the fast Fourier transform in space. As long as Nyquist–Shannon theorem is not violated, the method is exact in space (and the introduced numerical dispersion minimal). However, the time derivative is still approximated with finite differences that cause numerical error and dispersion. Nevertheless, fewer spatial grid points are required to achieve reasonable accuracy (e.g., the spatial discretization size $\Delta z = \lambda/10$ has been used\(^{135}\)).

Thereby, the computational workload is reduced. These advantages come at the price of a more complicated implementation. In particular, absorbing boundary conditions must be implemented in order to avoid the wrap-around effect. Furthermore, sharp material parameter changes and the implementation of sources are not trivial anymore.\(^{263}\)

### 7.2.2. Coupling Electric Field Updates and Density Matrix Updates

Since the electric field in Maxwell’s equations and the density matrix in the Bloch equations depend on each other, this coupling must be treated appropriately for any numerical method that solves Maxwell’s equations. Bidegáry distinguishes between strongly coupled methods\(^{237}\). The difference is the discretization of the density matrix in time and in relation to the electric field. Strongly coupled methods discretize the density matrix and the electric field at the same time value, weakly coupled methods apply a discretization which is staggered (a half time step difference between density matrix and electric field). In the following, we discuss various approaches to update the density matrix with different forms of coupling.

#### 7.2.3. Crank–Nicolson Scheme/Predictor–Corrector Method

The pioneering work by Ziolkowski et al.\(^{53,102}\) treats the Bloch equations with the Crank–Nicolson scheme

$$\hat{\rho}^{n+1} = \frac{1}{2} \hat{\rho}^{n} + \frac{1}{2} \left[ F^{n+1}(\hat{\rho}^{n+1}) + F^n(\hat{\rho}^n) \right]$$

(147)

where $n$ corresponds to the time $t_n = n\Delta t$, $\Delta t$ is the time step size, and $F(\hat{\rho}) = L(\hat{\rho}) + D(\hat{\rho})$ represents the right hand side of the Lindblad equation (3). Since this implicit scheme requires solving a linear system of equations at every time step, usually modifications are employed to reduce the numerical load, such as keeping the field at a fixed value while advancing the density matrix by a time step.\(^{207}\) A widely used variant is based on the predictor–corrector technique, where the update step first initializes $\hat{\rho}_{PC} = \hat{\rho}_n$, then executes the procedure

$$\hat{\rho}_{PC} \leftarrow \hat{\rho}_n + \Delta t \left[ \frac{1}{2\Delta t} F_{PC} + \frac{1}{2} \hat{\rho}_n \right]$$

(148)

four times, and finally assigns the result to the value $\hat{\rho}_{n+1} = \hat{\rho}_{PC}$.\(^{53,102}\)

In Figure 17a, the coupling of the method to the FDTD scheme is illustrated. It should be noted that this is a strongly coupled method and the electric field is updated with the same procedure (of course, $F$ is replaced with the right hand side of Ampere’s law) and in parallel to the density matrix update.

#### 7.2.4. Runge–Kutta Method

Several research groups use the fourth-order Runge–Kutta (RK) method to solve the Bloch equations.\(^{55,60,239,264}\) As illustrated in Figure 17b, the method is strongly coupled since electric field and density matrix are discretized at the same time steps. The exact procedure is not always described in related work, but can be outlined as follows.\(^{260}\) First, the electric field is updated using the standard FDTD update step. Then, the update of the density matrix using the rule

$$\hat{\rho}^{n+1} = \frac{1}{6} \hat{\rho}^{n} + \hat{\rho}^n_1 + 2\hat{\rho}^n_2 + 2\hat{\rho}^n_3 + \hat{\rho}^n_4$$

(149)

follows, where $\hat{\rho}^n_1 = F^n(\hat{\rho}^n)$, $\hat{\rho}^n_2 = F^{n+1/2}(\hat{\rho}^n + \Delta_t k_1/2)$, $\hat{\rho}^n_3 = F^{n+1/2}(\hat{\rho}^n + \Delta_t k_2/2)$, and $\hat{\rho}^n_4 = F^{n+1}(\hat{\rho}^n + \Delta_t k_3/2)$. Since the $F^n$ contains the electric field $E^n$ at time $t_n = n\Delta t$, not only the old and updated field values are required, but also the value at the half time step. The latter can be approximated by averaging between the old and the updated field value, that is, $E^{n+1/2} \approx \left( E^n + E^{n+1} \right)/2$. 

![Figure 17. Discretization and data dependencies of the finite-difference time-domain (FDTD) method combined with the a) predictor–corrector (PC), b) Runge–Kutta (RK), and c) matrix exponential (ME) method for the density matrix updates.](Image)
7.2.5. Matrix Exponential Methods

The methods of this group aim to solve the Bloch equations exactly for one time step. As illustrated in Figure 17c, the updates of electric field and density matrix are weakly coupled, that is, their updates are performed alternately. The density matrix update reads

$$\rho^{n+1/2} = \exp(\mathcal{F}^n \Delta t) \rho^{n-1/2}$$

(150)

where $\mathcal{F}^n$ may depend on the electric field $\mathbf{E}^n$ and $\exp(\mathcal{F}^n \Delta t)$ represents the exact solution of the Lindblad equation. After that, the standard FDTD update rule calculates $\mathbf{E}^{n+1}$ using $\mathbf{E}^n$ and $\rho^{n+1/2}$.

If an analytical expression for the solution superoperator $\exp(\mathcal{F}t)$ exists, this method is clearly the most accurate one. However, finding such an analytical expression is far from trivial. In fact, the exact form of the exponential depends on the representation. In Liouville or coherence vector representation described in Section 3.4, the solution superoperator has the form $\exp(Ft)$, where $F$ is a matrix. While this is straightforward to solve, the size of the matrix is in the order $N^2 \times N^2$ for a $N \times N$ density matrix. Since the exponential of a $N \times N$ matrix would generally need $O(N^3)$ operations, calculating the exponential in Liouville representation requires $O(N^3)$ operations and becomes unfeasible for large $N$.

In regular representation, a solution for the Lindblad equation must be found first. The Strang splitting technique\cite{Strang1968} can help here to separate the effects of the Liouvillian $\mathcal{L}$ and the dissipation superoperator $\mathcal{D}$. The solution for the Liouvillian requires the calculation of $\exp(-iH_1t\hbar)$, where the Hamiltonian $H$ is a $N \times N$ Hermitian matrix. The calculation requires $O(N^3)$ operations, which is still quite intensive.

The Strang splitting introduces an additional error of $O(\Delta t^2)$ in general. Furthermore, $\mathcal{F}$ is generally time dependent due to its dependence on the time-varying electric field, in which case the resulting matrix exponentials contain an integral in the exponent. Commonly, the integral is approximated using the midpoint rule. This leads to the conclusion that in reality the accuracy of matrix exponential methods is comparable to other approaches. Nevertheless, this group of methods preserves certain matrix properties and despite their limited performance they have attracted the focus of many research groups.

Several techniques have been applied in order to improve the performance of matrix exponential methods. The already mentioned Strang splitting has not only been used to allow analytical solutions, but also to separate the time dependent and time independent part of $\mathcal{F}$.\cite{Cayley1855,Magnus1954,Sylvester1868,Strang1968} This has the advantage that a part of the solution can be precalculated and applied at every time step, while for the remaining part, efficient evaluation techniques exist in some cases. For example, we discovered that the coherence vector representation leads to a real skew-symmetric matrix in the exponential. This expression can be evaluated efficiently using the generalized Rodrigues’ formula.\cite{ Rodrigues1840} Other techniques to calculate the matrix exponential have been applied in related work: an approximation based on the Cayley transform,\cite{Cayley1855,Magnus1954,Sylvester1868} Magnus expansion via Sylvester’s formula,\cite{Sylvester1868} diagonalization of the matrix,\cite{Diagonalization1997} the scaling and squaring method as well as a Krylov subspace method,\cite{Krylov1997} and Chebyshev polynomials.\cite{Chebyshev1852}

\subsection{7.2.6. Comparison of Numerical Methods for the Bloch Equations}

As already outlined above, the matrix exponential methods are the most computationally expensive ones. In fact, this was confirmed in a detailed investigation,\cite{Kraus1997} where both the Runge–Kutta and the predictor–corrector implementation outperformed the matrix exponential method. In this comparison, the predictor–corrector method demonstrated the best performance.

In terms of accuracy, Runge–Kutta methods have the highest order. However, the accuracy alone is not the crucial criterion. In particular, it was demonstrated that the Crank–Nicolson scheme does not preserve the positivity of the density matrix in the general case (at least when more than two energy levels are considered) and therefore might yield unrealistic results, for example, negative populations.\cite{Kraus1997} Furthermore, it was found that both the predictor–corrector and Runge–Kutta method yield negative populations in certain cases (e.g., long simulation end time combined with unfortunate choices for the time step size), while the matrix exponential method preserves the properties of the density matrix independent of the simulation settings.\cite{Kraus1997}

\subsection{7.2.7. Alternative Methods}

Besides the full-wave Bloch equations of the form Equation (17), related formalisms are used to model quantum systems interacting with a semiclassical optical field, requiring adapted numerical schemes which are often combined with the FDTD method for Maxwell’s equations. For example, MB simulations which replace the Bloch equations by an equivalent evolution equation for the polarization vector, Equation (72), require modified schemes adapted to the second-order differential form of Equation (72).\cite{Chen2000,Chen2004,Chen2005}

If the dissipation term in the Bloch equations can be neglected and the quantum system is in a pure state, the time evolution can be described in a simplified manner with the time dependent Schrödinger equation, Equation (1), for which suitable numerical schemes have been developed.\cite{Schrodinger1926,Schrödinger1926,Schrödinger1926b,Schrödinger1926c} In analogy to the MB equations, the Schrödinger and Maxwell’s equations can be combined to the Maxwell–Schrödinger approach, which is, for example, used to model nanoelectronic systems,\cite{Bernevig2005,Bernevig2006} or to describe the interaction of atoms with intense laser fields.\cite{Klaft2009,Klaft2010} As for the MB equations, such a coupled simulation complicates the numerical treatment, and various numerical schemes have been developed, for example, combining FDTD or transmission line matrix simulations of Maxwell’s equations with a spatial grid representation or eigenstate expansion of the wavefunction.\cite{Bernevig2005,Bernevig2006,Bernevig2008,Bernevig2009} In this context, a recent interest has been on algorithms preserving the symplectic structure of the Maxwell–Schrödinger equations, thus ensuring energy conservation of the coupled system.\cite{Klaft2009,Klaft2010}

\section{8. Inclusion of Further Effects}

\subsection{8.1. Local-Field Correction}

In principle, the current/polarization contribution of an individual quantum system at a given position can be directly...
represented in Maxwell’s equations by a point source,[239] without using ensemble averaging as in Section 4.1. However, the complexity of such an approach increases significantly with the number of quantum systems to be included.[239] Moreover, care must be taken that the field which drives the quantum system does not contain the divergent self-field contribution of the system itself, which further adds to the numerical load.[239,287] An alternative approach, which is especially suitable for a large ensemble of quantum systems as considered in this paper, is based on macroscopic MB equations. Rather than setting up Bloch equations for each of the quantum systems, the ensemble is here modeled by representative density matrices $\rho_d(x, t)$ distributed over the device volume, for example, placed on the spatial grid points, where $x$ is the macroscopic position coordinate. Likewise, Maxwell’s equations then contain the macroscopic current densities (see Section 4.1) and fields, defined as ensemble averages.

The local-field correction can, for example, lead to frequency shifts, and becomes relevant for densely spaced quantum systems, such as in tightly localized artificial quantum systems consisting of multiple semiconductor atoms (see Section 8.1.2).[289] It has been pointed out that local-field effects can be exploited as an additional design degree of freedom in nanostructures.[290]

8.1.1. Near-Dipole–Dipole Effects in Dense Media

The macroscopic field $\mathbf{E}$ comprises contributions of external sources as well as an internal contribution $\mathbf{E}_p$ due to the induced dipoles in the material, which is related to $\mathbf{P}_d$. In the following, we consider a medium such as a gas or crystal lattice which consists of a dense collection of atoms, molecules, or other quantum systems, as illustrated in Figure 18. The local field $\mathbf{E}_l$ at the position of the considered quantum system is determined by replacing the volume-averaged field $\mathbf{E}_p$ with the microscopic contribution $\mathbf{E}_{near}$ due to the nearby dipole moments, $\mathbf{E}_l = \mathbf{E} - \mathbf{E}_p + \mathbf{E}_{near}$. Based on a macroscopically large, but macroscopically small probe volume, which is conveniently chosen to be spherical, the macroscopic polarization contribution is obtained as $\mathbf{E}_p = -\mathbf{P}_d/(3\varepsilon_0)$. On the other hand, it can be shown that for dipoles arranged in a cubic lattice as illustrated in Figure 18, $\mathbf{E}_{near}$ vanishes for a particle on a lattice site, where the particle’s self-field is not included.[63,185] This yields $\mathbf{E}_l = \mathbf{E} + \mathbf{P}_d/(3\varepsilon_0)$, which is also approximately true for other reasonably isotropic media and completely random arrangements, such as amorphous media or gases.[63,185] Retardation effects are here negligible since the probe volume diameter is assumed to be much smaller than the optical wavelength.[63,289] For two-level systems where the polarization is given by Equation (71), the local-field corrections can thus be included in the Maxwell–Bloch equations by formally substituting $\Sigma = d_{12} \mathbf{E}/\hbar$ with

$$\Omega_1 = d_{12} \mathbf{E}_l/\hbar = \Omega + 2\omega_0 \Re \{\rho_{21}\}$$

(151)

in Equation (67)[292] where the static Lorentz shift

$$\omega_1 = d_{12}^2 \eta_{3D}/(3\hbar \varepsilon_0)$$

has the dimension of frequency. Here, we have assumed a real-valued $d_{12}$ for simplicity. Applying the RWA, we obtain Equation (73) where we have to substitute $\hat{\Sigma}$ by

$$\hat{\Omega}_1 = \hat{\Omega} + 2\omega_0\eta_{21}$$

(152)

which changes Equation (73a) but not Equation (73b) since there the local-field correction term cancels out.[63]

If the quantum systems are embedded in a host medium, such as dopant ions in a crystal, they interact not only with particles of the same species, but also with those of the host material, and the local-field correction must be suitably extended. Accordingly, above approach has been generalized to a dense collection of two-level atoms embedded in a linear, potentially dispersive, and absorptive host medium,[291] and to multicomponent media in general.[296] Furthermore, above concept can be straightforwardly extended to more than two levels.[295]

We note that above correction to the MB equations has mainly been considered for ensembles of atoms or molecules, where typically much higher number densities are obtained than for artificial systems such as quantum dots. This model has enabled the analytical[296] and numerical[297–299] investigation of numerous effects, such as solitonic and ultrashort pulse propagation or optical switching. For artificial, tightly localized quantum systems, local-field effects are typically governed by the depolarization field, as discussed below.
The depolarization factor \( L_d = d_L N d_{12} / d_{12} \), with \( 0 \leq L_d \leq 1 \) accounts for the anisotropy of the object, such as an ellipsoidal quantum dot, and becomes \( L_d = 1/3 \) for spherical geometries.\(^{[64]}\)

The resulting equations have been used for both analytical\(^{[300]}\) and numerical\(^{[290,300,301]}\) studies of local field effects in quantum dots.

### 8.2. Inhomogeneous Broadening

Homogeneous broadening is naturally considered in the Bloch equations. This can best be seen from the steady-state solution in RWA, Equation (128), yielding a Lorentzian lineshape with the width given by the dephasing rate of the corresponding transition (see Equations (129) and (132) as well as Figure 13b). In addition, inhomogeneous broadening arises if the optically active medium consists of quantum systems with slightly different resonance frequencies,\(^{[49,109]}\) as, for example, frequently arises in ensembles of quantum dots due to size fluctuations. Another example is Doppler broadening in a gas,\(^{[302]}\) caused by the Doppler shift due to the thermal motion of the atoms or molecules. For a given transition between two states \(|i\rangle\) and \(|j\rangle\), the distribution of the resonance frequency \(\omega_{ij}\) is commonly described by a distribution function \(g_{ij}(\omega_{ij} - \bar{\omega}_{ij})\) with \(\int_{-\infty}^{\infty} g_{ij}(\omega) d\omega = 1\), where \(\omega_{ij} - \bar{\omega}_{ij}\) is the deviation from the average resonance frequency \(\bar{\omega}_{ij}\). For thermal Doppler broadening, \(g_{ij}\) is given by a Gaussian distribution

\[
g_{ij}(\omega_{ij} - \bar{\omega}_{ij}) = \frac{1}{\sqrt{2\pi}\sigma_{ij}} \exp\left(-\frac{(\omega_{ij} - \bar{\omega}_{ij})^2}{2\sigma_{ij}^2}\right) \tag{153}\]

In this case, the standard deviation becomes \(\sigma_{ij} = \left(\bar{\omega}_{ij}/c\right)(k_b T/m)^{1/2}\), where \(k_b\) is the Boltzmann constant, \(T\) indicates the temperature, and \(m\) is the mass of the atom or molecule.\(^{[302]}\) The Gaussian distribution, Equation (153), is also frequently used as a generic model if the distribution of resonance frequencies is not exactly known, for example, to describe above mentioned inhomogeneous broadening in ensembles of quantum dots due to size fluctuations.\(^{[303]}\) If the individual quantum systems contain more than one relevant optical transition with distributed resonance frequencies, in principle joint distribution functions have to be used.

Numerically, the full-wave or RWA Bloch equations, Equation (17) or (43), have to be solved separately for each possible value of the resonance frequency (or each possible combination of resonance frequency values if the individual quantum systems contain more than one relevant optical transition).\(^{[261]}\) This requires discretizing the distribution function into a finite number of \(N_{bins}\) bins with resonance frequencies \(\omega_{ij}, s = 1..N_{bins}\). Each of these bins is represented by a corresponding quantum system subensemble with density matrix \(\rho_{ij}^{(s)}\), where the fraction of carriers \(p_i\) is proportional to the weight of that bin and \(\sum_i p_i = 1\). The polarization current density is then obtained from a generalized version of Equation (48).

\[
\mathbf{J}_p = \pi_3 \sum_{i,j} d_{ij} \sum_s p_i \tilde{\mathbf{a}}_i \rho_{ij}^{(s)} \tag{154}\]
In SVAAn, the polarization amplitude is given by a generalized form of Equation (64).

\[ \mathbf{P} = 2n_{3D} \sum_{a_i j} d_{ij} \sum_s p_i a_i^s \]  

(155)

For certain broadening mechanisms, such as fluctuations in quantum dot size, also \( d_{ij} \) can in principle vary which could be considered by introducing a quantity \( d_{ij}^s \) in Equations (154) and (155) in analogy to \( a_i^s \), but this effect is usually neglected.

In certain cases, inhomogeneous broadening can also be considered in analytical solutions of the MB equations based on the RWA. These usually invoke the factorization ansatz, which assumes that nonresonant systems with a finite frequency detuning \( \Delta = \omega_0 - \omega_{12} \neq 0 \) essentially respond in the same way to the optical field as the resonant ones, apart from a detuning dependent amplitude \( F(\Delta) \). In Section 6.1.2, this approach has been demonstrated in the context of self-induced transparency.

8.3. Noise

Noise in optoelectronic devices arises, for example, from spontaneous emission and from processes in the semiconductor host, such as lattice vibrations. Noise and fluctuations can generally be included into the semiclassical MB equations by adding stochastic terms.\(^{[140,145]} \) Numerically, the stochastic terms are typically implemented by using a pseudorandom number generator to obtain uncorrelated, Gaussian distributed random numbers for every grid point.\(^{[173,185]} \) The MB equations, complemented by these additional stochastic terms, are then numerically solved as discussed in Section 7, for example, with an FDTD-based approach.\(^{[173,185]} \) The MB equations and stochastic terms are systematically obtained from the quantum Langevin equations,\(^{[171,187]} \) which are then represented by equivalent stochastic c-number equations,\(^{[173,188,189]} \) that is, evolution equations for operator expectation values with additional stochastic terms.

Spontaneous emission obviously plays an important role in optoelectronic devices. While the resulting recombination can simply be included by nonlinear rate terms for the carrier occupations in Equation (17b) or (43b),\(^{[180,183]} \) the noise contribution is not included in the MB model due to its semiclassical nature. This effect can however be considered in terms of a Gaussian white noise source in the optical propagation equation.\(^{[173,181,182]} \) In different models, dipole fluctuations are also included by adding Langevin noise terms not only to the propagation equation, but also to Equation (17a) for the off-diagonal density matrix elements.\(^{[180,184]} \) By virtue of the fluctuation–dissipation theorem, a decay of populations, coherences, or the optical field is generally accompanied by fluctuations, and an MB equation model which includes such decay-induced fluctuations has been presented.\(^{[188,189]} \) Furthermore, an extension of the stochastic c-number approach to incorporate nonclassical effects has been discussed.\(^{[189]} \)

9. Application to Optoelectronic Devices

For interband optoelectronic devices based on semiconductor bulk or quantum-well media, the conduction and valence band states are given by \( |c, k \rangle \) and \( |v, k \rangle \), respectively. Here, \( k \) is the 3D crystal wavevector in bulk media or the 2D in-plane wavevector for quantum well structures (see Section 3.3). In the following, we define \( \rho_{c,k} \) and \( (1 - \rho_{c,k}) \) as the electron occupation probability of a conduction band state \( |c, k \rangle \) and a valence band state \( |v, k \rangle \), respectively, that is, \( \rho_{c,k} \) corresponds to the hole occupation probability of a valence band state. Restricting ourselves to direct bandgap semiconductors in a two-band approximation and using that the optical transitions are \( k \) conserving, as can for quantum wells be seen from Equation (24),\(^{[165]} \) the Bloch equations, Equation (17), become

\[
\dot{\rho}_{c,k} = -i\omega_{c,k} \rho_{c,k} - i\Omega_k \left( \rho_{c,k} + \rho_{v,k} - 1 \right) + \left[ \partial_{c,v} \rho_{c,k} \right]_{\text{col}} \tag{156a}
\]

\[
\dot{\rho}_{v,k} = i\Omega_k \rho_{v,k}^* - i\rho_{c,k}^* \rho_{v,k} + \left[ \partial_{v,c} \rho_{v,k} \right]_{\text{col}} \tag{156b}
\]

with \( \alpha = c, v \). Here, the sum over \( k \) implicitly also includes summation over the two possible spin orientations. This equation applies to quantum wells, where the carriers are treated as a 2D gas, as well as bulk media. The dissipation processes are here included by general collision terms \( [\partial_{c,v} \rho_{c,k}]_{\text{col}} \) and \( [\partial_{v,c} \rho_{v,k}]_{\text{col}} \). These can be modeled on a microscopic level, in particular accounting for carrier–carrier and carrier–phonon scattering, or under certain approximations by relaxation rate terms similar to those in Equation (17).\(^{[185,186]} \) Many-body Coulomb interactions can be taken into account based on the Hartree–Fock approximation, which results in the so-called semiconductor Bloch equations, which have the form of Equation (156) but feature renormalized transition and Rabi frequencies

\[
\omega_{c,v,k} = \frac{1}{\hbar} E_{c,v,k} - \frac{1}{\hbar} \sum_{q \neq k} V_{k-q} \left( \rho_{c,q} + \rho_{v,q} \right) \tag{157a}
\]

\[
\Omega_k = \frac{d_{c,k} E}{\hbar} + \frac{1}{\hbar} \sum_{q \neq k} V_{k-q} \rho_{c,q} \tag{157b}
\]

leading to a coupling of the states with different \( k \) through the time dependent renormalization terms.\(^{[185,186,189]} \) In Equation (157a), \( E_{c,v,k} \) is the energy of free electron–hole pairs, which can in a simple model be described as

\[
E_{c,v} = \frac{1}{2} h^2 k^2 \left( \frac{1}{m_c^*} + \frac{1}{m_h^*} \right) + E_B \tag{158}
\]

Here, \( E_B \) denotes the bandgap energy, or for quantum wells the energy difference between the electron and hole state energies. Furthermore, \( m_c^* \) and \( m_h^* \) are the electron and hole effective masses, assuming a parabolic dispersion relation near the conduction and valence band edges, respectively. \( V_q \) is the Coulomb potential in Fourier representation, which is in a bulk with probe volume \( V_p \) and background permittivity \( \varepsilon_0 \) given by \( V_q = \varepsilon_0 V_p / 2 \varepsilon_0 \varepsilon_q V_p \), and in a quantum well structure with in-plane cross section \( S \) by \( V_q = \varepsilon_0 V_p / (2 \varepsilon_0 \varepsilon_S S) \). Screening effects,
which result from the response of the other carriers and weaken the potential, are then incorporated as corrections to the Hartree–Fock equations in the form of a modified $V_p$. Summing in Equation (48) over the initial and final states $|i\rangle = |c, k\rangle$ and $|j\rangle = |v, q\rangle$ where we consider that the total number density of electron–hole pairs is given by

$$n_{cv}(t) = V_p^{-1} \sum_k \rho_{c,k}(t) = V_p^{-1} \sum_k \rho_{v,k}(t)$$  \hspace{1cm} (159)

and using the $k$ conservation of optical transitions, $d_{ij} = d_{cv,k} \delta_{k,q}$, we obtain for the polarization term

$$\partial_t P_q = V_p^{-1} \sum_k (d_{cv,k} \rho_{c,k} + c.c.)$$  \hspace{1cm} (160)

With Equation (160), Equations (156) and (157) can be coupled to the Maxwell equations, Equation (44), resulting in the semiconductor Maxwell–Bloch equations. These equations have been extensively used for the simulation of semiconductor lasers and related devices.[11,58] Furthermore, they have been adapted to the modeling of quantum wire structures[11,58] as well as graphene[11,58] and carbon nanotubes.[119]

As stated in Section 1, a further discussion of this model is beyond the scope of this paper. Rather, we will focus here on approaches which reduce above two-band model to macroscopic two- or $N$-level Bloch equations. As a first step, the collision terms in Equation (156) are modeled by relaxation rate terms similar to those in Equation (17). Extending the rate equation model Equation (9) to states $|\alpha, k\rangle$ results in a Boltzmann-type collision term for the populations, which can in consideration of Pauli blocking be written as

$$[\partial_t \rho_{c,k}^\alpha]_{col} = -\rho_{c,k}^\alpha (W_{v\alpha}^c + W_{\alpha v}^c) + (1 - \rho_{c,k}^\alpha) \left( W_{v\alpha}^c + W_{\alpha v}^c \right)$$  \hspace{1cm} (161)

Here, $\beta \neq \alpha$, that is, for the conduction band collision term ($\alpha = c$), we have $\beta = v$, while $\beta = c$ for $\alpha = v$. The Boltzmann rates are related to the electron transition rates of Section 2.2.1 by $W_{v\alpha}^c = \sum_k f_{c,k} - f_{v,k}$ and $W_{\alpha v}^c = \sum_k f_{c,k} - f_{v,k}$, where $f_{c,k}$ denotes the electron occupation probability, that is, $f_{c,k} = \rho_{c,k}$ and $f_{v,k} = 1 - \rho_{c,k}$. For example, spontaneous emission and carrier–phonon scattering can be modeled by Equation (161) with adequately chosen transition rates $r_{c,v}$, while the inclusion of carrier–carrier interactions beyond Hartree–Fock effectively requires rates which themselves depend on the carrier distribution.[58] Furthermore, modeling the dephasing in analogy to Equation (12), we obtain

$$[\partial_t \rho_{c,k}^\alpha]_{col} = -\gamma_{c,v} \rho_{c,k}^\alpha$$  \hspace{1cm} (162a)

$$[\partial_t \rho_{v,k}^\alpha]_{col} = \Gamma_{v\alpha,k} - r_{v\alpha,k} \rho_{v,k}^\alpha + \Gamma_{\alpha v,k} - r_{\alpha v,k} \rho_{c,k}^\alpha$$  \hspace{1cm} (162b)

In Equation (162a), $\gamma_{c,v}$ indicates the dephasing rate. Rearranging the contributions in Equation (161), Equation (162b) is obtained, where the first two terms on the right hand side with $\beta \neq \alpha$ describe interband processes, while the other two terms model the intraband transitions. Here, $r_{v\alpha,k} = W_{v\alpha,k}^c$ denotes the interband (for $\alpha' = \beta$) or intraband (for $\alpha' = \alpha$) recombination rate due to nonradiative transitions and spontaneous emission. Furthermore, $\Gamma_{v\alpha,k} = (1 - \rho_{c,k}) W_{\alpha v}^c$ describes the filling of state $|\alpha, k\rangle$, and can for $\alpha' = \beta$ be interpreted as a pump rate, where carriers are induced, for example, by an injection current or optical pumping. Summation of Equation (161) or Equation (162b) over $k$ yields $\sum_k [\partial_t \rho_{c,k}^\alpha]_{col} = \sum_k [\partial_t \rho_{v,k}^\alpha]_{col}$, as expected from Equation (159). In more detail, for the intraband contributions we have

$$\sum_k (\Gamma_{v\alpha,k} - r_{v\alpha,k} \rho_{c,k}) = 0$$  \hspace{1cm} (163)

while the interband terms fulfill

$$\sum_k r_{v\alpha,k} \rho_{v,k} = \sum_k r_{v\alpha,k} \rho_{c,k}$$  \hspace{1cm} (164)

To obtain compact two-level Bloch equations, we assume a $k$ independent dipole matrix element $d_{\alpha, k} = d_{\alpha, k}^{\alpha}$, in Equation (157a) and ignore the renormalization contribution, yielding the usual definition $\Omega_{\alpha} = \hbar^{-1} d_{\alpha, k}^{\alpha} E$. Summing Equation (156b) over $k$ yields with Equations (159), (162b), (163), and (164) and $P_{cv} = V_p^{-1} \sum_k \rho_{cv}^\alpha$

$$\partial_t n_{cv} = i \Omega_{cv} P_{cv}^* + \Gamma_{12} - \gamma_{11} n_{cv}$$  \hspace{1cm} (165)

For electrical pumping, the injection rate $\Gamma_{12} = \sum_k \Gamma_{v\alpha,k}$ with $\alpha = c, \beta = v$ or $\alpha = v, \beta = c$ can be modeled as $\Gamma_{12} = \eta V_p^{-1} 1/e$, where $\eta$ and $l$ denote the injection efficiency and current, respectively. The recombination rate $\gamma_1$ which includes nonradiative and spontaneous transitions, is obtained by averaging over the carrier distribution, $\gamma_1 = \sum_k r_{v\alpha,k} \rho_{c,k} / n_{cv}$. Proceeding in a similar manner for Equation (156a) by neglecting the $k$ dependence of $\omega_{cv,k}$ is not feasible, due to the problems arising from the summation over $\rho_{c,k} + \rho_{v,k} - 1$. Various strategies have been developed to circumvent this problem.[58–60] Here, we follow the approach by Yao et al.[60] formulated in the framework of the RWA. Thus, we start by introducing the slowly varying field envelope $E$ and the transformed off-diagonal elements defined in Equations (41) and (42), respectively. Furthermore, assuming a $k$ independent Rabi frequency $\Omega = \hbar^{-1} d_{\alpha, k} E$, Equation (156a) yields with Equation (162a)

$$\partial_t n_{cv} = (i \Delta_k - \gamma_{cv} n_{cv}) n_{cv} - \frac{1}{2} \Omega (\rho_{c,k} + \rho_{v,k} - 1)$$  \hspace{1cm} (166)

where $\Delta_k = \omega_{c,k} - \omega_{cv,k}$ with $\omega_{cv,k}$ given by Equation (157a). In the framework of semi-phenomenological macroscopic MB equation models, the renormalization term is often neglected.[58,60] The $k$ dependence can be modeled with Equation (158) or a more sophisticated description. Dividing Equation (166) by $(\alpha_k - \gamma_{cv})$, summing over $k$ and defining $p_{cv} = V_p^{-1} \sum_k n_{cv,k}$, we obtain

$$\partial_t p_{cv} = \frac{i}{2} \frac{\tau_1}{\tau_2} \Omega n_{cv} - \tau_1^{-1} p_{cv}$$  \hspace{1cm} (167)
where we have furthermore used Equation (159) and introduced the complex parameters \( r_1 \) and \( r_2 \) with

\[
V_p^{-1} \sum_k \left( \rho^{c,k} + \rho^{a,k} - 1 \right) \gamma_{cv,k} - i \Delta_k = r_1 n_{cv}
\]

\[
V_p^{-1} \sum_k \left( \rho^{a,k} \right) \gamma_{cv,k} - i \Delta_k = r_2 p_{cv}
\]

Equation (167) and Equation (165) in RWA,

\[
\partial_t n_{cv} = \frac{i}{2} \left( \Omega p_{cv}^* - \Omega^* p_{cv} \right) + \Gamma_{12} - \gamma_1 n_{cv}
\]

constitute macroscopic Bloch equations for interband transitions in bulk semiconductor and quantum well systems. In order to obtain a Maxwell–Bloch model, Equations (167) and (169) can be coupled to the optical propagation equation in SVA, Equation (62), where the RWA polarization term is obtained from Equation (73) as \( P = 2d_c P_{cv} \). The parameters \( r_1 \) and \( r_2 \) introduced in Equation (168) can, for example, be evaluated numerically, or by fitting to experimental data.[80] In this context, it has been found that \( r_1 \) and \( r_2 \) can be treated as independent of the optical intensity, but that especially \( r_2 \) shows pronounced dependence on \( n_{cv} \), which should be considered in the model,[80] and also allows a phenomenological reintroduction of renormalization effects.

9.2. Quantum Well Intersubband Devices

Intersubband devices, such as QCLs,[7] quantum cascade detectors,[8,9] and quantum well infrared photodetectors (QWIPs),[10] commonly utilize optical intersubband transitions between quantized energy levels in the conduction band \( \Gamma \) valley of a multiple quantum well structure. The Maxwell–Bloch model has been extensively applied to such devices, especially for the dynamic modeling of QCLs. The quantized states \( |\psi_i, k\rangle \), also referred to as subbands, are characterized by their wavefunction \( \psi_i(x) \) where \( i \) is the subband index, and in-plane wavevector \( k = [x, y, 0]^T \). These states are commonly found by solving the 1D effective mass Schrödinger equation, obtained from inserting the ansatz Equation (19) into Equation (20), for the quantum well potential \( V(x) \). As mentioned in Section 3.3.1, band bending due to space charge effects is usually considered by solving the coupled Schrödinger–Poisson equation system,[125,126] and also nonparabolicity effects, which play a role especially in mid-infrared devices, can be included.[127,128] These calculations yield the eigenenergies \( \varepsilon_i \) and wavefunctions \( \psi_i \), and thus the transition frequencies \( \omega_{ij} = h^{-1} (\varepsilon_i - \varepsilon_j) \) and the dipole matrix elements, Equation (25), as input for the Bloch equations. We again choose the semiconductor Bloch equations as a starting point, with a form analogous to Equation (156). Due to the typically low doping levels of QCLs, the Hartree–Fock renormalization effects in Equation (157) have been found to be relatively small,[121] and also Pauli blocking only plays a secondary role. Furthermore, we can assume \( k \) independent transition frequencies \( \omega_{ij} \) at least for terahertz QCLs, where the energetic level spacings are smaller than in mid-infrared QCLs and thus the subbands have nearly parallel dispersion relationships. Under these assumptions, summing over \( k \) yields Bloch equations of the form Equation (17), where we have used that the dipole matrix element is \( k \) conserving, and introduced intersubband scattering rates \( r_{j \to i} \) which are related to the generally \( k \) dependent rates \( r_{j \to q \to i} \) by \( r_{j \to i} = \sum_k r_{j \to q \to i} k^2 \rho_{ij}^q \). Assuming either moderate temporal variations of the intersubband electron distribution \( \rho_{ij}^q \) or a moderate \( k \) dependence of the rates, the \( r_{j \to i} \) are approximately given by

\[
r_{j \to i} = \sum_k r_{j \to q \to i} k^2 \rho_{ij}^q / \sum_k \rho_{ij}^0 
\]

Here, \( \rho_{ij}^0 \) describes the steady-state electron distribution in the subband.[322] Notably, the intersubband electron distributions in QCLs can often be reasonably well approximated by Fermi–Dirac or Maxwell–Boltzmann distributions, parametrized by subband electron temperatures which can significantly exceed the lattice temperature.[119,123] By contrast, the off-diagonal density matrix elements generally vary strongly with time, and no clearly defined concept exists how the \( k \) averaging should be performed to obtain an effective dephasing rate \( \gamma_j \) from a relaxation term of the form Equation (162a), \( \langle \hat{b} \hat{b} \rangle = -\gamma_j k \rho_{ij}^0 k \). This especially matters if the ratio \( \rho_{ij}^0 / \rho_{ji}^0 \) has a strong \( k \) dependence, as is the case for significantly different subband electron temperatures or highly nonthermal distributions.[322] Often, an average over the population inversion of the involved subbands is applied,[101,124]

\[
\gamma_{ij} = \sum_k \gamma_{j,k} \rho_{ik}^0 / \sum_k |\rho_{ik}^0 - \rho_{ij}^0 k|
\]

and a comparison to an alternative way of averaging has yielded similar results for terahertz QCLs.[98] Apart from very few exceptions based on the full-wave MB equations,[61,106,325] typically a two-level model is employed. In the case of mid-infrared QCLs, where nonparabolicity effects play a more important role, an approach similar to Equation (167) can be envisaged. The transition and dephasing rates are usually empirically chosen, or extracted from fits to experimental data. Alternatively, they can be calculated from Equations (170) and (171) based on the Hamiltonians of the relevant scattering mechanisms, such as electron–electron interactions, scattering with acoustic and longitudinal optical phonons, as well as impurity, interface roughness and alloy scattering.[119,322] Here, the use of dissipation rates derived from steady-state models is consistent with the Markovian and time-homogeneous character of the Lindblad dissipator, which provides the basis for the Bloch equations. The corresponding scattering rates are typically evaluated based on Fermi’s golden rule,[119] while the associated pure dephasing rates can be obtained from Ando’s model.[98,327,328]

For QCLs, the MB equations have primarily been used to study ultrashort pulse generation by mode-locking,[10,120,122,232,233,326,129,332] and the closely related formation of coherent instabilities,[202,208,333] as well as the generation of frequency combs.[62,97,322,334,335] In detail, it has been found that coherent multimode instabilities result in the emergence
of sidebands around the original longitudinal mode, giving rise to broadband multimode operation.\cite{202,208} Furthermore, active mode-locking has been investigated where short pulses are generated by modulating the laser current at the cavity roundtrip frequency, yielding good agreement between simulations and measurements.\cite{329–332} Also the possibility of realizing passive mode-locking in QCLs has been theoretically explored.\cite{30,120,122,232,233} Here, pulse formation is obtained by adding saturable absorption regions, where SIT mode-locking, discussed in Section 6.1.2, constitutes a special variant. Besides, frequency comb operation has been studied, where an equidistant line spectrum is generated, which serves as a ruler in the frequency domain for spectroscopic and sensing applications. Here, a perturbative treatment of the MB equations imposing a comb-like spectrum has been employed,\cite{334,335} as well as full numerical simulations.\cite{62,97,122} In most of above works, spatial hole burning has been considered based on Equations (123) and (124), as it considerably affects the QCL dynamics. In addition, various other effects have been implemented which can play an important role for mode-locked and frequency comb operation in QCLs, such as tunneling across thick barriers\cite{62,97,122} and group velocity dispersion due to the waveguide and bulk semiconductor material.\cite{62,97,233,322,335,336} For optical excitation on very short timescales, memory effects become important and the presuppositions of the Lindblad approach are too restrictive, requiring the use of more complex models such as the quantum-kinetic schemes.\cite{147–159}

As mentioned above, MB simulations have, for example, been used to model frequency comb operation of QCLs, identifying four-wave mixing as the primary comb forming mechanism and explaining experimentally observed features.\cite{62,97,322,334,335} In Figure 20, a comparison between simulation and experiment is presented for the power spectrum.\cite{62} generated by a THz QCL for frequency comb generation.\cite{340} Good agreement is found; in particular, a splitting of the comb spectrum into a high and a low frequency lobe is observed in both simulation and experiment. Also the simulated temporal dynamics agrees well with experiment. In Figure 21, the simulated and measured instantaneous optical power in the high and low frequency lobe of the comb is shown.\cite{62} Again, good agreement between theory and experiment is obtained, confirming the validity of the MB model. In particular, the temporal switching behavior between the two lobes is reproduced in the simulation.

9.3. Quantum Dot Devices

Due to the strong carrier localization and discrete energy spectrum resulting from the 3D confinement in QDs, they enable lasers and laser amplifiers with excellent gain, threshold, temperature, and dynamic characteristics.\cite{1–3} While these devices rely on interband optical transitions, also the possibility has been studied to exploit intraband transitions similarly as in QCLs to obtain lasing in the mid-infrared or terahertz regime.\cite{300,341–343} Furthermore, intraband transitions between bound electron or hole states (or from bound to continuum states) have been employed for quantum dot infrared photodetectors.\cite{11–13}

In contrast to bulk semiconductors and quantum well or wire structures which feature a continuum of states due to the free carrier motion in at least one dimension, the QD possesses a discrete set of energy eigenstates. Thus, the application of phenomenological models based on generic discrete-level MB equations appears to be especially justified for QD systems. Phenomenological two-level MB equations have been employed for a large range of applications based on QDs. This includes studies of the spatiotemporal dynamics\cite{344–346} and SIT mode-locking\cite{121} in QD lasers, FDTD-based MB simulations of QD photonic-crystal-cavity lasers,\cite{60} and QDs coupled to a nanoparticle or cavity.\cite{347–349} Furthermore, three-level MB equations have been used, for example, to study EIT,\cite{648} soliton propagation,\cite{350} or all-optical switching\cite{351} in QD structures, and also four-level models have been developed.\cite{152,176}

Optoelectronic applications employing large ensembles of QDs are often fabricated utilizing self-assembly of the QDs on top of an initial quasi-2D semiconductor layer, which is referred to as wetting layer, as sketched in Figure 22.a. The resulting structure is subsequently covered by another layer of suitable semiconductor material. The wetting layer effectively forms a quantum well, which serves as a reservoir for the carriers. The thus obtained QD layer forms the basis of various devices such as QD lasers (see Figure 22b), where commonly multiple layers are stacked on top of each other to increase the optical gain.

In Figure 23, a schematic energy diagram of the wetting layer and a QD is shown. A description of the QD dynamics based on

![Figure 20](image1.png)

**Figure 20.** Optical comb spectrum of a terahertz QCL, as obtained from a) simulation and b) experiment.

![Figure 21](image2.png)

**Figure 21.** Instantaneous optical power in the high and low frequency lobe as obtained from a) simulation and b) experiment.
the semiconductor Bloch equations, Equations (156) and (157), features renormalized transition and Rabi frequencies due to many-body Coulomb interactions.\textsuperscript{[303,312,353]} These renormalization effects are often neglected so that the conventional Bloch equations, Equation (17), can be used as a starting point, which are frequently supplemented by a detailed model for Coulomb scattering and other scattering mechanisms in the dissipation term.\textsuperscript{[303,311]} In the following, the QD conduction ($\alpha = c$) and valence ($\alpha = v$) band states are labeled by an index $i$. Furthermore, as described in Section 8.2, variations in QD size result in distribution of resonances, and the associated inhomogeneous broadening is included by dividing the QDs in corresponding subensembles $s$ containing a fraction $p_s$ of QDs. The Bloch equations, Equation (17), thus have to be adapted by replacing the density matrix elements $\rho_{ij}$ with $\rho_{s\alpha,i,j}$ for pairs of states $|\alpha, i\rangle$ and $|\alpha', j\rangle$, where we write for compactness $\rho_{s\alpha,i,j} = \rho_{s\alpha,i,j}^{(i)}, \rho_{s\alpha',i,j} = \rho_{s\alpha',i,j}^{(i)}$, and $\rho_{s\alpha,i,j} = \rho_{s\alpha,i,j}^{(f)}$. For the dipole matrix element vectors $d_{ij}$, frequencies $\omega_{ij}$, and dephasing rates $\gamma_{ij}$, we proceed analogously. Similarly as for Equation (156), the $\rho_{s\alpha,i,j}^{(i)}$ are taken as the hole occupation probability of the $i$th QD valence band level, that is, matrix elements $\rho_{\alpha,i,j}$ in Equation (17) referring to the electron occupation probabilities of QD valence band states have to be substituted by $(1 - \rho_{\alpha,i,j})$. Apart from the coherent light–matter interaction, incoherent carrier transitions in QD systems mainly occur due to carrier–carrier scattering which gives rise to Auger-type processes, as well as carrier–phonon interactions and spontaneous photon emission.\textsuperscript{[303,310]} Rate equation terms of the form Equation (9) with phenomenologically chosen parameters are frequently used to model incoherent transitions in QD systems.\textsuperscript{[60,121,248,344,346,347]} For a more detailed modeling, it must be taken into account that important dissipative processes in QDs depend on the occupations of two or more states, and that Pauli blocking is not included in Equation (9). This can be addressed by using an empirical nonlinear rate equation model,\textsuperscript{[207,354]} or based on a microscopic treatment.\textsuperscript{[303,310,311,353]} For high pump currents, Auger processes, where two carriers scatter from their respective initial to final levels, involving QD and wetting layer states, constitute the dominant scattering process.\textsuperscript{[303]} This includes scattering of two electrons or holes, as well as mixed processes involving an electron transition in the conduction band and a hole transition in the valence band. The associated change of the occupation $\rho_{\alpha,i,j}$ is in the following represented by a generic intraband collision term $[\hbar \rho_{\alpha,i,j}]_{\text{intra}}$,\textsuperscript{[303]} which can be generalized to also include other scattering-induced intraband carrier transitions, for example, due to electron–phonon interactions. Additionally, spontaneous electron–hole recombination is typically taken into account as an important interband process, which depends on the occupations of the initial and the final state. Within this model, the dissipation terms in Equation (17b) are substituted by the more general ansatz for incoherent processes\textsuperscript{[303]}

$$[\hbar \rho_{\alpha,i,j}]_{\text{intra}} = [\hbar \rho_{\alpha,i,j}]_{\text{intra}} - \sum_j A_{v,i,j} \rho_{v,i,j}^{(f)} \rho_{\alpha,i,j}$$

(172)

with the spontaneous recombination coefficient $A_{v,i,j}$. The Lindblad dephasing rate approach of the form Equation (12), as also used in Equation (17a), has been argued to be generally well suited to model dephasing in QDs.\textsuperscript{[311]} The dephasing rates can be calculated based on microscopic models for carrier–carrier and carrier–phonon scattering,\textsuperscript{[311,355–357]} or are phenomenologically chosen.\textsuperscript{[248,303,312,351]}

Considering that $[\hbar \rho_{\alpha,i,j}]_{\text{intra}}$ contains intra-QD transitions as well as carrier exchange between the wetting layers and QD states, this term not only depends on the occupations of the QD states involved, but also on the carrier densities in the wetting layers. Thus, for a closed carrier transport model, the Bloch equations have to be extended by equations for the wetting layers, which can be modeled by\textsuperscript{[303]}

$$\partial_t w_{\alpha} = \frac{J_{\alpha}}{e} - A_{\alpha} w_{\alpha} - 2n_{2D} \sum_i \rho_{s\alpha,i,j}^{(f)} [\hbar \rho_{\alpha,i,j}]_{\text{intra}}$$

(173)
Here, \( n_s \) denotes the overall carrier sheet densities in the wetting layers, that is, \( n_s \) is the total number of conduction band electrons in all wetting layers divided by the area \( S \) of a wetting layer, and \( u_s \) is defined analogously for the valence band. \( J_p \) denotes the electric pump current density. Furthermore, \( n_{2D} \) is the overall QD sheet density, and the factor 2 accounts for the spin degeneracy of the QD states. \( A_s \) in Equation (173) is the rate coefficient for spontaneous band–band recombination in the wetting layers. Sometimes the carrier injection from the bulk to the quantum well wetting layers is modeled by additional equations.\(^{358}\) For self-assembled quantum dot structures, the wetting layers can be considered in an analogous manner.\(^{21,339}\)

The extended Bloch equations. Equations (17), (172), and (173), are then coupled to Maxwell’s equations, Equation (44), by the polarization current density for inhomogeneously broadened media given in Equation (154),

\[
J_q = \frac{n_{2D}}{d_g} \sum_{a,\alpha} \sum_{i,j} \sum_{s} n_s (1 - \delta_{\alpha \alpha'} \delta_{ij}) \partial_t \rho_{q,a,i}^{\alpha,\alpha'} (174)
\]

with the thickness of the gain medium \( d_g \). Here, the term \( (1 - \ldots) \) compensates for the fact that the electron occupation probabilities of QD valence band states are in our density matrix convention given by \( (1 - \rho_{q,i}^{\alpha}) \). QD lasers and amplifiers usually operate in TE mode, due to the character of the eigenstates for the QD shapes and strains obtained with the widely employed Stranski–Krastanov growth mode.\(^{360}\) A corresponding 1D MB model can be obtained by combining the extended Bloch equations with Maxwell-type equations for TE operation, Equation (92), where the finite overlap of the QD active region with the mode profile is considered by the field confinement factor, Equation (88). The contribution of the spontaneous emission processes in Equation (172) to the optical field is in most cases neglected, but can be considered as discussed in Section 8.3.

For interband QD devices, optical intersubband transitions can be neglected. The QD interband dipole matrix elements are given by Equation (22). As discussed in Section 3.3.2, for the uppermost valence and lowest conduction band states, in good approximation only optical interband transitions between states with equal quantum numbers are allowed, and the corresponding envelope wavefunction overlap in Equation (22) is \( \langle \phi_i | \phi_j \rangle \approx 1 \).\(^{146,147}\) In fact, for these states close to the band edge, the index \( i \) is typically associated with a single quantum number,\(^{303}\) due to the typically small aspect ratio of QDs. Under above assumptions, the Bloch equations simplify to

\[
\partial_t \rho_{c,v,i}^{\alpha} = -i \omega_{c,v}^{\alpha} \rho_{c,v,i}^{\alpha} + \hbar^{-1} d_{c,v}^{\alpha} (1 - \rho_{c,v,i}^{\alpha} - \rho_{v,c,i}^{\alpha}) E - \gamma_{c,v}^{\alpha} \rho_{c,v,i}^{\alpha} \]

\[
\partial_t \rho_{c,v,i}^{\alpha} = 2 \hbar^{-1} \gamma_{c,v}^{\alpha} (d_{c,v}^{\alpha} \rho_{c,v,i}^{\alpha} E + [\hbar \rho_{c,v,i}^{\alpha}]_{\text{intra}} - K_{c,v}^{\alpha} \rho_{c,v}^{\alpha} \rho_{v,c}^{\alpha} \]

with \( \alpha = c, v \) and \( d_{c,v}^{\alpha} \) has been approximated by an \( s \) and \( i \) independent value \( d_{c,v} \).\(^{303}\) For a closed description of the carrier dynamics, Equation (175) is again supplemented by Equation (173).\(^{303}\) The radiative and nonradiative transitions taken into account in the resulting model are illustrated in Figure 23. The RWA can be applied in the usual manner, as described in Section 3.5. The MB model has been demonstrated to yield good agreement with experimental results for QD lasers and amplifiers, and to be instrumental in interpreting the experimental findings. For example, the ultrafast gain dynamics in a QD amplifier as well as the spatiotemporal dynamics and emission characteristics of a QD laser were experimentally and theoretically studied.\(^{361}\) Furthermore, based on MB simulations of ultrashort laser pulse propagation in a QD amplifier, it could be confirmed that the experimentally observed reshaping was in part due to coherent light–matter interaction.\(^{21,22}\)

As discussed in Section 5.3.2, longitudinal spatial hole burning, that is, the formation of an inversion grating due to the standing wave pattern in a Fabry–Pérot resonator, is automatically included in full-wave MB simulations. Assuming that tunneling between adjacent QDs can be neglected, the degradation of the inversion grating is governed by carrier diffusion in the wetting layers, which can be modeled by adding to Equation (173) a diffusion term of the form Equation (120).\(^{306,307}\)

**10. Conclusion and Outlook**

The goal of this review has been to discuss in detail the underlying theoretical framework of the MB model, its extension and adaption to certain application areas and types of nanostructures, as well as special analytical solutions and suitable numerical methods. Apart from the intuitive appeal of the model and its adaptability, the relative compactness of the Bloch equations make them highly suitable as an efficient quantum model for the material polarization in computational electrodynamics. As shown in Section 7, their representation as a system of ordinary differential equations in time, where the position coordinates only enter as parameters, allows an efficient coupling to numerical schemes for Maxwell’s or related propagation equations, such as the finite-difference time-domain method. This compact form of the Bloch equations is enabled by a mostly phenomenological treatment of dissipation based on the Lindblad formalism and restriction to classical optical fields as well as discrete energy levels. Fully microscopic descriptions of light–matter interaction in a semiconductor, such as the semiconductor MB equations shortly discussed in Section 9.1,\(^{65,66}\) illustrate the limitations of semi-phenomenological Bloch equations, and can serve as a starting point to develop improved compact Bloch equations. As an example, this strategy has been used to model the carrier dynamics in a semiconductor structure with a quasi-continuum of energy levels in the conduction and valence band by macroscopic discrete-level Bloch equations,\(^{67-69}\) as discussed in Section 9.1.

The main requirement for computational models is generally to combine numerical efficiency with accuracy, predictability, and versatility. In this context, detailed microscopic theories can quickly become very computationally demanding, which renders them impractical for applications such as device design.\(^{362}\) Thus, a major goal is to further improve the quantitative accuracy and adaptability of the macroscopic MB equations by extending the model accordingly, however, without substantially increasing its numerical complexity. This implies that its general form as a system of a few ordinary differential equations should not be compromised.

Probably the main limitation of the Bloch equations is the phenomenological implementation of dissipation based on the Lindblad formalism. As shortly discussed in Section 9.3, an empirical treatment of certain processes, such as Pauli blocking...
or carrier–carrier scattering, requires a generalization to non-linear models. Here, special care must be taken to preserve the properties of the density matrix guaranteeing its physical character, which has, for example, been achieved by suitably extending the Lindblad formalism.[73]

As mentioned in Section 2.3, the Lindblad model is only realistic from a microscopic point of view if the memory decay of the environment occurs on a faster timescale than the coherent system dynamics and relaxation processes.[75,81] Although the macroscopic MB equations often work surprisingly well on the verge of, or even outside, this microscopic validity range, advanced quantitative modeling requires going beyond the Markovian approximation in such cases. An ad hoc extension of the Lindblad approach is obtained by replacing the memory kernel. Which has, for example, been achieved by suitably extending the Lindblad formalism. [73] In this case, it is necessary to treat the populations in the usual manner and include memory effects only for dephasing, which requires substituting the dephasing terms $|d_{ij}\rangle\langle d_{i}'j'|$ in Equation (12) with $-\gamma_{ij} d_{ij} \rho_{ij} \rho_{ij}'$.[166] Since the characteristic time and functional dependence of the memory kernel, such as Gaussian or exponential, depend on the underlying scattering mechanism. It should be pointed out that master equation models with memory effects do not necessarily require convolution integrals,[78] and that memory kernel master equations can even usually be cast into a time-local form.[79,83,166] Thus, a promising approach toward a more generalized treatment of dissipation is to start with the Lindblad equation in the form Equation (4), and to generalize the matrix $D_{ij}$ given in Equation (6) for an arbitrary set of Lindblad operators. As already mentioned in Section 2, time dependent Lindblad operators $L(t)$, corresponding to time-varying dissipation rates in Equations (8) and (11), are unproblematic.[78,79] Any further generalization of $D_{ij}$ comes at the price of potentially unphysical results. One example is the occurrence of temporarily negative rates in Equations (8) or (11), which indeed introduces memory effects into the Lindblad equation.[79,366–370] In the construction of such a model, care should be taken to avoid unphysical behavior, for example, by adding certain constraints.[79,166] Furthermore, a widely used model of the form Equation (4) is the Redfield equation, which is derived from microscopic considerations, that is, a perturbative treatment of a quantum system weakly coupled to the environment.[371,372] In this case, $D_{ij}$ corresponds to the generally time-dependent[73] Redfield tensor, which is directly related to the system–environment coupling and environment Hamiltonians.[174] The main advantages of the Redfield model are its strong connection to microscopic physics, and to some extent the inclusion of short-term memory effects.[173,375] However, in its commonly used form, the Redfield equation does not guarantee positivity of the density matrix which can lead to negative state occupations. In practice, the emergence of this unphysical behavior appears to be a minor problem,[376–378] and can also be cured.[173,179]

Finally, applying the Lindblad formalism to a suitably extended state space, a non-Markovian evolution with arbitrarily long memory times and strong initial correlations can be described.[380] This is achieved by representing the reduced system density matrix $\rho_i$, with dimension $N$, as a sum of a certain number $M$ of positive matrices $\rho_i$, that is, $\rho_i = \sum \rho_i$, where the traces of the $\rho_i$ must add up to one. Then, a big block diagonal density matrix $\rho$ with dimension $MN$ is constructed from the $\rho_i$, and the evolution of $\rho$ is modeled by a Lindblad equation for the extended system, where the operators are required to preserve the block diagonal form of $\rho$. This leads to $M$ coupled evolution equations for each $\rho_i$ where the dynamics is now defined by $M$ arbitrary Hermitian operators $H_i$ and $M^2$ sets of arbitrary dissipation operators $(L_{ij}^{(1)}, \ldots, L_{ij}^{(M)})$. In this way, although the dynamics of $\rho$ is Markovian, the model can describe a highly non-Markovian evolution of $\rho_i$, while intrinsically preserving the physical properties of $\rho$. An interesting subcase is when the evolution equations of the $\rho_i$ are decoupled, that is, $L_{ij}^{(1)} = L_{ij}^{(2)} \delta_{ij}$. In this case, the evolution of each $\rho_i$ is described by an equation of the Lindblad form Equation (3), but still a non-Markovian dynamics of $\rho_i$ is obtained. Of course, for $M = 1$, the standard Markovian Lindblad dynamics is recovered.

Appendix: List of Symbols and Acronyms

| Symbol | Description |
|--------|-------------|
| A      | Magnetic vector potential |
| $\alpha$ | Spontaneous emission coefficient |
| $A_{\text{eff}}$ | Effective mode area |
| $A_q$ | Quantum active region cross section |
| $a$ | Power loss coefficient |
| $c$ | Vacuum speed of light |
| $D$ | Diffusion coefficient |
| $D$ | Displacement field |
| $D_{ij}$ | Dissipation superoperator |
| $d_i$ | Dipole operator |
| $d_{ij}$ | Dipole matrix element vector |
| $E$ | Electric field |
| $E_{\text{sc}}$ | Slowly varying amplitude of $E$ |
| $E_{\text{sc}}$ | $\mathbf{E}$ for forward/backward propagating field |
| $E_{\text{g}}$ | Bandgap energy |
| $E_{\text{f}}$ | Eigenenergy of level $i$ |
| $E_{\text{g}}$ | Fourier amplitude of waveguide E-field |
| $E_{\text{T}}$ | Transverse dependency of $E$ |
| $E_{\text{T}}$ | Electromagnetically induced transparency |
| $e$ | Elementary charge |
| $e_i$ | Polarization direction of electric field |
| $F$ | Modal field distribution |
| $F_{\text{g}}$ | $F_i$ Wavefunction of semiconductor state $i$, $F_i = \phi_i u_{\text{i}}$ |
| $\text{FDTD}$ | Finite difference time-domain |
| $f_{\pm}$ | Forward/backward normalized polarization amplitude |
| $g$ | Power gain coefficient |
| $g(\omega)$ | Distribution function of resonance frequencies |
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