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Computational Optoelectronics of Semiconductor Nanostructures Including Many-Body Effects

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The linear and nonlinear optical properties of semiconductors are strongly influenced by the Coulomb interaction among the photoexcited carriers. Within the framework of the semiconductor Bloch equations such many-body effects can be described on the basis of a microscopic theory. In this article, we briefly review our recent contributions to two specific topics. First, the coherent optical generation of charge and spin currents and their subsequent decay via scattering processes is discussed. As a second example, the spatially-inhomogeneous optical properties of hybrid structures which consist of photonic crystals and semiconductor nanostructures are described. Many of the numerical results have been obtained using massively parallel computer programs which were run on the IBM p690-Cluster Jump in Jülich.

1 Introduction

The analysis of the optical and electronic properties of semiconductors and, in particular, semiconductor nanostructures is of great current interest. On the one hand, one can study in these systems questions which are of relevance in the area of fundamental physics, i.e., many-body and non-equilibrium effects, ultrafast dynamics, coherent phenomena, influence of disorder, etc. On the other hand, semiconductors and semiconductor nanostructures are useful for a great variety of applications including optoelectronic devices.

A microscopic theoretical description of the optical properties of semiconductors has to properly describe the light field, the material excitations, and their interaction. When the electronic system is excited by the light field, electrons are raised energetically to the previously unoccupied conduction band and so-called holes are generated in the valence band. Since these quasi-particles are charged, their mutual Coulomb interaction gives rise to a many-body problem. Within the framework of the semiconductor Bloch equations a number of important many-body effects can be computed on a microscopic theoretical basis[1,2]. These equations describe the dynamical evolution of electronic distributions and coherences during and after the photoexcitation. By numerically solving this high-dimensional set of coupled nonlinear differential equations one obtains the macroscopic optical polarization which appears as a source term in Maxwell's equations and thus determines the light-matter interaction.

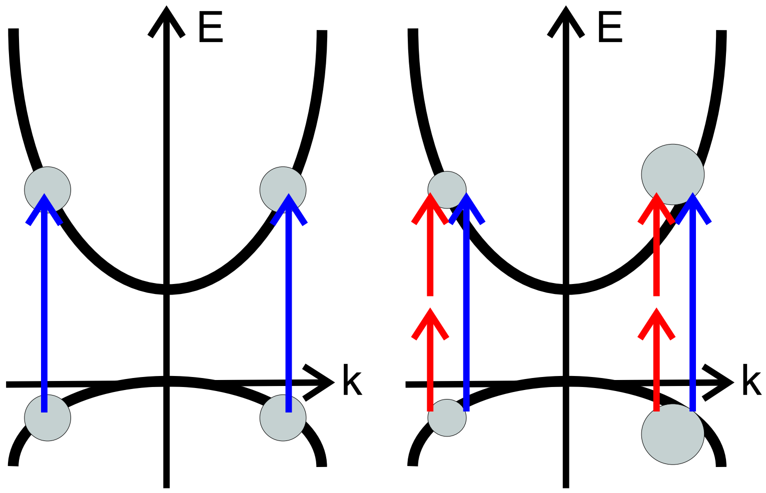

Figure 1. Schematical drawings of optical interband excitations in a two-band model. Left: A single field with frequency 2ω resonantly generates electrons and holes above the band gap of a semiconductor $E_{\rm gap}$. In this case, the excitation is symmetric in k-space. Right: The incident field consists of two frequencies ω and 2ω satisfying $\hbar\omega < E_{\rm gap} < 2\hbar\omega$. In this case, it is possible to create excitations which are not symmetric in k-space, i.e., correspond to a finite current, since the initial and final states are connected by two pathways. The direction and the magnitude of the photoinduced current can be controlled coherently by adjusting the phase difference between the two field components.

In this brief review, we describe our recent contributions to two specific topics. For further details of the theoretical approach and additional information we have to refer the reader to the cited articles and the literature cited therein. In the first example, see Sect. 2.1, the coherent optical generation of charge and spin currents and their subsequent decay via scattering processes is analyzed. As a second example, the spatially-inhomogeneous optical properties of hybrid structures consisting of photonic crystals and semiconductor nanostructures are described in Sect. 2.2.

2 Examples

2.1 Coherent Optical Generation and Decay of Charge and Spin Currents

Recently, the coherent control of electronic excitations in semiconductors by sequences of optical laser pulses has received great attention. For example, it has been predicted[3] that it should be possible to generate photocurrents in semiconductors on ultrashort time scales via the excitation with two light beams with frequencies ω and 2ω satisfying $\hbar\omega < E_{\rm gap} < 2\hbar\omega$, where $E_{\rm gap}$ is the band gap energy. This effect has been observed[4] and is illustrated schematically in Fig. 1.

A few years later, it has been predicted that basically the same type of interference scheme can also be employed to create pure spin currents which are not accompanied by any charge current[5], see Fig. 2. The existence of such spin currents generated on ultrafast time scales has been confirmed experimentally[6,7]. They could, in particular, be useful for possible future applications in the area of spintronics.

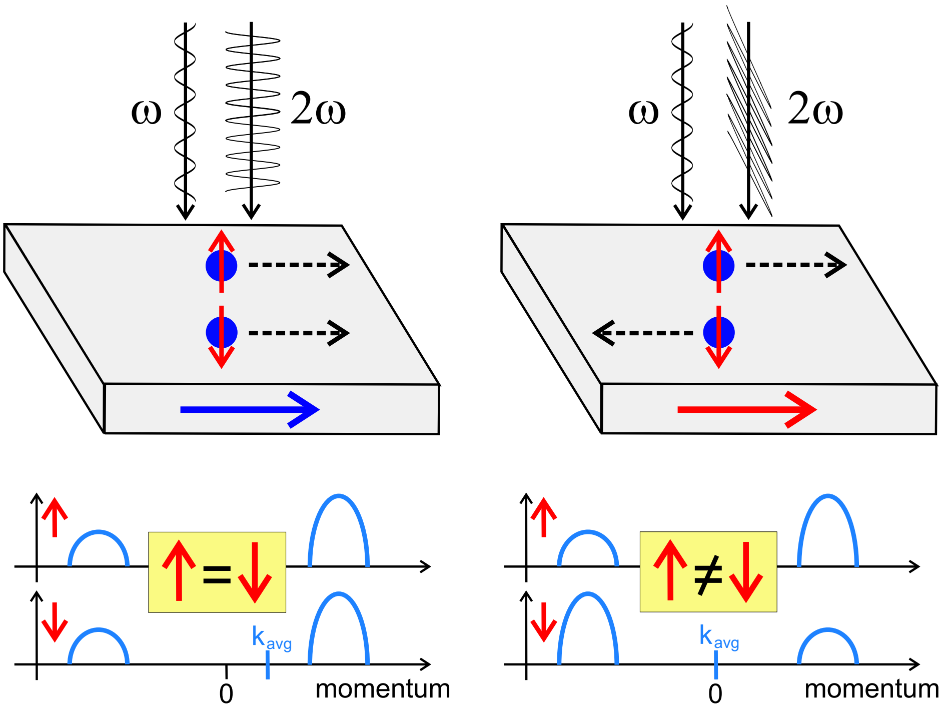

Figure 2. Schematical illustration of the coherent optical generation of currents. Left: (Right:) By using linear parallel (perpendicular) polarization directions of the ω and the 2ω beams a charge (spin) current is injected. When a charge current is generated, both spins are excited identically, i.e., $n^e_{\uparrow,k} = n^e_{\downarrow,k}$, and the excitations carry a nonvanishing average momentum $k_{\rm avg}$. For the case of a spin current, the distributions of the two spins satisfy $n^e_{\uparrow,k} = n^e_{\downarrow,-k}$ and thus the momentum averaged over both spins vanishes.

In Ref. 8, we have presented and analyzed a microscopic many-body theory at the quantum-kinetic second Born-Markov level which is capable of describing the dynamical generation, the coherent evolution, and the decay of charge and spin currents. Our approach is based on the semiconductor Bloch equations[1,2] and includes light-field-induced intraband and interband excitations nonperturbatively and beyond the rotating wave approximation, excitonic effects, as well as correlation contributions arising from the carrier LO-phonon coupling and the Coulomb interaction which describe scattering processes.

Figure 3 shows the time-dependence of the electron and hole distributions of a quantum well in k-space. The short laser pulses generate carriers with a combined excess energy of 150 meV above the band gap. Due to their smaller mass most of this kinetic energy is given to the electrons. Immediately after the photoexcitation, the electron and hole distributions are very similar, since the optical transitions are diagonal in k-space. Due to the quantum interference between the ω and 2ω components of the field, the distributions are larger for positive k_x than for negative k_x. Therefore, this situation corresponds to a current in x-direction. In the course of time, the distributions relax towards quasi equilibrium, i.e., towards the band edges. In the limit of long times, due to their larger mass the distribution of the holes is wider than that of the electrons.

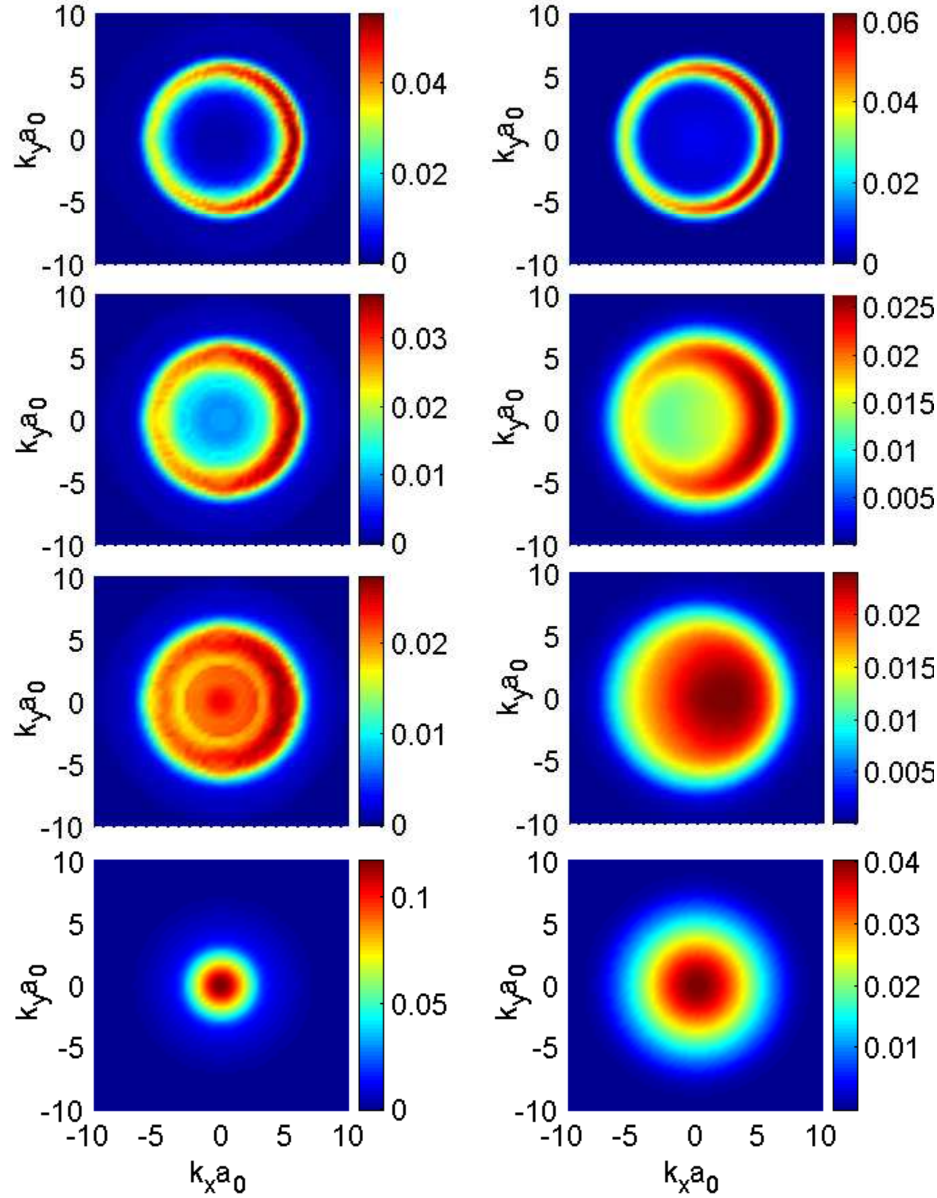

Figure 3. Left (right) column: Contour plots of the electron (hole) distributions in a quantum well in $\mathbf{k}$-space at t =50, 100, 150, and 400 fs, respectively. The incident pulses have a duration of 20 fs and the amplitudes of the two fields are $A_\omega = 2A_{2\omega} = 108A_0$, with $A_0 = E_0/ea_0 \approx 4$ kV/cm, where E_0 is the exciton Rydberg and a_0 the exciton Bohr radius. The excitation frequency is chosen such that $2\hbar\omega$ is 150 meV above the band gap, the density of photoinjected carriers is $N = 10^{11}$ cm^{-2}, and the temperature is $T = 50$ K. Taken from Ref. 8.

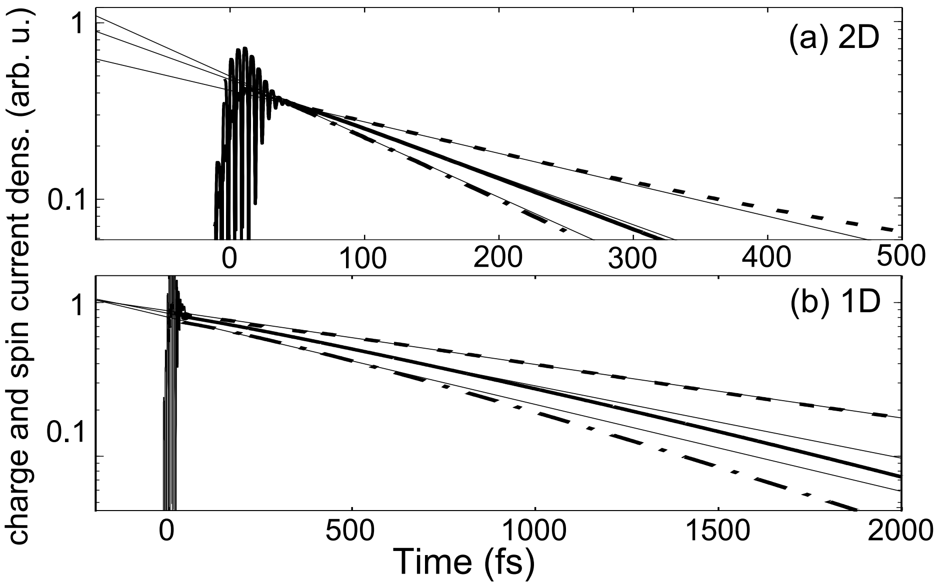

Figure 4. (a) Time-dependent charge (solid) and spin (dash-dot) currents of a quantum well for the same parameters as in Fig. 3. Also shown is the identical decay of both currents if only carrier LO-phonon scattering is considered (dashed). The thin solid lines represent exponential decays with time constants of 240, 155, and 125 fs, respectively. (b) Same as (a) for a quantum wire. The density of the photoinjected carriers is $N = 5 \times 10^5$ cm^{-1} and the other parameters are the same as in (a). The thin solid lines represent exponential decays with time constants of 1250, 900, and 740 fs, respectively. Taken from Ref. 8.

Figure 4(a) demonstrates that for the considered excitation conditions the dynamical evolution of the currents is influenced by both carrier LO-phonon and carrier-carrier scattering. If only carrier LO-phonon scattering is considered, the charge and spin currents decay similarly. This decay is not exponential, however, its onset can be approximated by an exponential decay with a time constant 240 fs. Including also carrier-carrier scattering in the analysis, speeds up the decay of both currents. Additionally, we find that *the spin current decays more rapidly than the charge current*. This effect can be understood by considering that the excitation of a charge current corresponds to identical electron distributions for the different spins, see Fig. 2. Therefore, the average momentum of the electron system is finite. Since carrier-carrer scattering only exchanges momentum among the carriers, the finite average momentum cannot be reduced by this process. The situation is, however, different when a spin current is excited. In this case, the opposite electron distributions for the two spins correspond to a vanishing total electronic momentum, see Fig. 2. Consequently, Coulomb scattering can exchange and thus relax the photoexcited momenta of the spin-up and spin-down electrons.

Figure 4(b) shows that qualitatively similar results are obtained for quantum wires. However, since the phase space is smaller in one dimension, the scattering is reduced and the decay times are longer than in two dimensions. Additional investigations of the dependence of the currents on the intensities of the incident laser pulses can be found in Ref. 8.

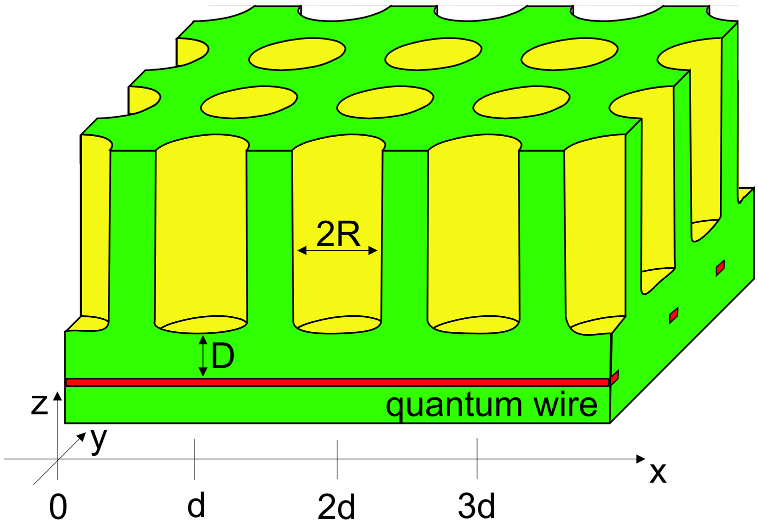

Figure 5. Schematical drawing of the considered structure which consists of an array of semiconductor quantum wires in the vicinity of a two-dimensional photonic crystal. The photonic crystal has a finite thickness and is made of periodically arranged air cylinders which are surrounded by a dielectric medium. Taken from Ref. 15.

2.2 Optical Properties of Semiconductor Photonic-Crystal Structures

A periodic wavelength scale dielectric structuring strongly influences the transverse part of the electromagnetic field. Dielectric photonic crystals can be used to design the dispersion of the electromagnetic field modes, i.e., so-called photonic band structures[9–12]. Important aspects of the light-matter interaction can be modified with these structures and, furthermore, a suitable tailoring of the field modes may improve the properties of various optoelectronic devices.

The dielectric structuring influences, however, also the longitudinal part of the electromagnetic field, i.e., the Coulomb interaction. This results in a space dependence of the band gap and the exciton energies in a nearby semiconductor nanostructure which follows the periodicity of the photonic crystal[13,14].

In Ref. 15, we have analyzed the optical gain properties of such spatially-inhomogeneous semiconductor photonic-crystal structures. The developed theoretical approach provides a self-consistent solution of the dynamics of the electromagnetic field and the material excitations in the framework of coupled Maxwell semiconductor Bloch equations which include many-body interactions on the Hartree-Fock level.

The considered structure consists of an array of quantum wires in the vicinity of a two-dimensional photonic crystal of finite thickness, see Fig. 5. Shown in Fig. 6. are density-dependent optical absorption and gain spectra. For small densities, two excitonic absorption peaks are visible. The lower one is associated with positions underneath the dielectric part of the photonic crystal whereas the higher one originates from positions underneath the air cylinders. With increasing density, the height of both peaks decreases due to bleaching. However, the rate of change for the energetically lower peak is larger. This

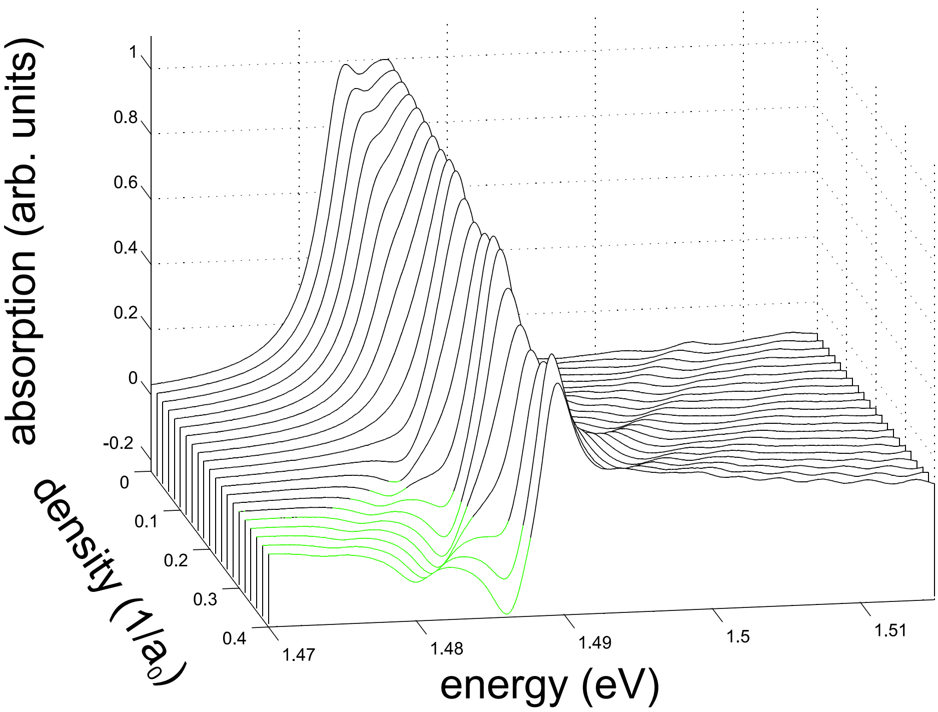

Figure 6. Density-dependent absorption/gain spectra for an array of wires that is separated by $D = 0.2a_0$ from the photonic crystal with air cylinder radius $R = 2.65a_0$. The presence of negative absorption, i.e., optical gain, is highlighted by changing the lines from black to green. Taken from Ref. 15.

is due to the fact that because of the spatially-varying band gap the carriers accumulate at positions underneath the dielectric and avoid the regions underneath the air cylinders. As a result the sign of the absorption at the lower peak becomes negative, i.e., optical gain is present, in a range of densities where the higher peak is still absorbing. A detailed analysis shows that in this spatially-inhomogeneous structure the transition from absorption to gain occurs at an approximately 20% smaller density than in a structure which is in a homogeneous dielectric environment[15].

Besides the gain, we have also studied nonlinear optical properties and electronic wave-packet dynamics of spatially-inhomogeneous semiconductor photonic-crystal structures[16]. Furthermore, a strong enhancement of the optical gain has been found in structures consisting of one-dimensional photonic crystals and semiconductor quantum wells[17].

3 Summary

The two examples presented here demonstrate that many-body effects strongly influence the optoelectronic properties of semiconductors. Many of our numerical results on the examples discussed here and also on other topics were obtained using massively parallel computer programs which were run on the IBM p690-Cluster Jump in Jülich.

Acknowledgments

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