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THE WAVE PACKET STUDY OF EXCITON DYNAMICS IN THE ZnSe–ZnTe QUANTUM WELL

P. Bała

Institute of Physics, N. Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland

In this paper we perform a detailed study of the formation and the dynamics of the exciton in the ZnSe/ZnTe quantum well taking into account two-particle nature of the process. The electron–hole interaction is included in the model through the electrostatic potential, which results in a nonlinear coupling of the electron and hole equations of motion. The coupled time-dependent Schrödinger equation describing the electron and hole dynamics is integrated numerically. The detailed dynamics of the excitonic electron–hole pair in the quantum well is presented for different uniform electric field applied across the structure.

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The exciton dynamics has been a topic of great interest in the recent years. The improvement of device fabrication technology and of measurement techniques allows nowadays for investigations of different aspects of the exciton dynamics in the bulk crystals and in various quantum structures [1, 2]. So far, resonant optical pumping was used to create spatially coherent quantum well excitons [3]. Such systems seem also to be interesting for the future device applications. The development in the time-resolved experiments allows also for the investigation of the short time dynamics of the excitons in semiconductors. The strong interest is in the formation process and early dynamics of the excited electron–hole which can be probed by the ultrafast optical spectroscopy [4–6].

A proper theoretical description of the exciton formation requires advanced techniques which disallow the usage of the standard stationary approach. The investigation of the formation of the electron–hole pair requires an individual description of the electron and hole and proper treatment of their interactions. The electron–hole coupling is essential for the exciton formation and cannot be neglected.

In this paper we perform a detailed study of the formation and dynamics of excitons in a ZnTe/ZnSe/ZnTe quantum well taking into account two-particle nature of the process. In the present approach, both the electron and the hole are treated in the full time-dependent formalism developed previously for the electrons [7].

In order to study dynamics of the exciton in the quantum well we need to solve the time-dependent Schrödinger equation (1) associated with the Hamiltonian of the spinless exciton in the heterostructure region [8]

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Phi(r_\mathrm{e}, r_\mathrm{h}) = H\Phi(r_\mathrm{e}, r_\mathrm{h}), \tag{1}$$

where r_e, r_h are electron and hole positions. Denoting the electron and hole effective masses by m_e^* and m_h^* the electron–hole Hamiltonian can be described as follows:

$$H = \left[-\frac{\hbar^2}{2m_\mathrm{e}^*}\frac{\partial^2}{\partial z_\mathrm{e}^2} + V_\mathrm{e}(z_\mathrm{e})\right] + \left[-\frac{\hbar^2}{2m_\mathrm{h}^*}\frac{\partial^2}{\partial z_\mathrm{h}^2} + V_\mathrm{h}(z_\mathrm{h})\right]$$
$$-\frac{\hbar^2}{2\mu_{xy}}\nabla_{xy}^2 + V_{\mathrm{e-h}}(\rho, r_\mathrm{e}, r_\mathrm{h}), \tag{2}$$

where μ_{xy} is the reduced electron–hole mass in $x-y$ plane and ρ is the relative electron–hole distance in the $x-y$ plane. The electron–hole interaction $V_{\mathrm{e-h}}$ is described by the Coulomb potential. Assuming that total wave function Φ can be separated into motion along z axis and the in-plane motion, the Schrödinger equation for the motion along the growth direction is obtained by the integration with respect to the ρ [8, 9]

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(z_\mathrm{e}, z_\mathrm{h})$$
$$= \left[-\frac{\hbar^2}{2m_\mathrm{e}^*}\frac{\partial^2}{\partial z_\mathrm{e}^2} + V_\mathrm{e}(z_\mathrm{e}) - \frac{\hbar^2}{2m_\mathrm{h}^*}\frac{\partial^2}{\partial z_\mathrm{h}^2} + V_\mathrm{h}(z_\mathrm{h}) + W(z_\mathrm{e} - z_\mathrm{h})\right]\Psi(z_\mathrm{e}, z_\mathrm{h}). \tag{3}$$

The coupling term $W(z_\mathrm{e} - z_\mathrm{h})$ contains Coulomb repulsion and in-plane motion of the exciton. The Schrödinger equation (3) can be simplified introducing a factorization $\Psi(z_\mathrm{e}, z_\mathrm{h}) = \Psi_\mathrm{e}(z_\mathrm{e})\Psi_\mathrm{h}(z_\mathrm{h})$. The set of coupled one-dimensional equations is then obtained

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi_\mathrm{e}(z_\mathrm{e}) = \left[-\frac{\hbar^2}{2m_\mathrm{e}^*}\frac{\partial^2}{\partial z_\mathrm{e}^2} + V_\mathrm{e}(z_\mathrm{e}) + W_\mathrm{h}(z_\mathrm{e})\right]\Psi_\mathrm{e}(z_\mathrm{e}), \tag{4}$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi_\mathrm{h}(z_\mathrm{h}) = \left[-\frac{\hbar^2}{2m_\mathrm{h}^*}\frac{\partial^2}{\partial z_\mathrm{h}^2} + V_\mathrm{h}(z_\mathrm{h}) + W_\mathrm{e}(z_\mathrm{h})\right]\Psi_\mathrm{h}(z_\mathrm{h}). \tag{5}$$

The equations are solved together since the term $W_i(z) = \int \Psi_i^2(z') \times W(z - z')\mathrm{d}z'$ couples electron and hole wave functions Ψ_e and Ψ_h. The coupling potential can be calculated analytically assuming exponential decay of the wave function for the in-plane motion of exciton [8].

The main interest is in exciton dynamics in type I superlattices, which can be effectively used for fabrication of blue emitting devices. The detailed study was performed for the exciton formation in the ZnTe/ZnSe rectangular quantum well of the width 50 Å. The barrier height for the electron movement is 2 eV, and the electron effective mass in the quantum well $m_\mathrm{e}^* = 0.17m_0$, while the hole effective mass is set to 1 ($m_\mathrm{h}^* = 1.00m_0$). The quantum well potentials $V_\mathrm{e}(z_\mathrm{e})$ and $V_\mathrm{h}(z_\mathrm{h})$ contain, except for the rectangular square potential also the potential of external uniform electrostatic field applied along the growth direction: eE_iz_i (i = e, h). In

practice, the potential energy surface is additionally deformed by the terms $W_i(z)$ which describe electron–hole coupling. One should note that coupling depends on the actual charge distribution in both the valence and conduction bands (Fig. 1) and it changes in time. Therefore the coupling term must be evaluated at each time step.

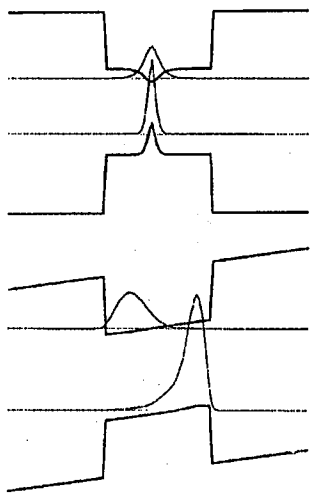

Fig. 1. The potential of the quantum well without (upper) and with (lower) applied uniform external electrostatic field. The modification of the potential forced by the electron–hole interaction is also included. The electron and hole wave functions are plotted for the time 1.0 ps.

The coupled one-dimensional nonlinear equations of motion for the conduction (4) and valence (5) bands are solved numerically using the grid methods applied before to the investigation of electron dynamics in the time dependent potential with nonlinear terms [7, 10].

The time step $\Delta t = 0.25$ fs and mesh size $\Delta x = 1.2$ Å are chosen to obtain high accuracy. We have assumed that the electron–hole pair is created at a time $t = 0$ in the middle of the quantum well and the initial wave functions of both the electron and the hole have Gaussian shapes with the width of 16 Å. When no external uniform potential is applied, the created exciton is stable and both carriers do not change their position. However, the width of the both electron and hole wave functions changes. Fast oscillations are observed, together with a constant, exponential change of the wave function dispersion. At $t = 0.2$ ps after the creation of the electron–hole pair the system reaches the stationary state and both oscillations and constant sweep of the wave packet width are no longer observed. The final width of the Ψ_e is larger than the width of Ψ_h which reflects a stronger localization of the hole in the quantum well due to its higher effective

mass. Because of the fact that an exciton is created in the middle of the quantum well, the coherent movement of the electron–hole pair is not observed.

When an electron–hole pair is not created in the center of the well (in the particular case 5.2 Å away from the center of the quantum well) the changes in the wave packet width are associated with the movement of the created pair towards the center of the well. However, due to the electron–hole interaction, the exciton stops 2 Å before the center of the well is reached. All the time the movement of the electron and hole is correlated although oscillations of the electron–hole distance are observed.

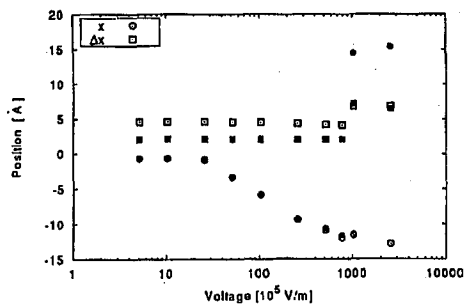

Fig. 2. Position of the center of the electron and hole wave functions (open and filled circles, respectively), and its width (open and filled squares) at the time 1.0 ps for different values of the applied external electric field.

The external electrostatic field applied across the structure modifies the quantum well potential, and the electron–hole pair, even created in the middle of the quantum well, moves. At a time 0.4 ps after the excitation the created pair stops at a new position, shifted from the middle of the quantum well. The final position, measured after 1 ps depends on the strength of the applied external field. For the weak fields (lower than 2×10^6 V/m) the center of the pair remains almost in the same place (Fig. 2). For the more intense fields, exponential change of the equilibrium position is observed. The electrostatic field stronger than 7×10^7 V/m destroys the created electron–hole pair. The movement of both particles is uncorrelated, and electron and hole wave functions are localized in the opposite parts of the quantum well. In this case, an increase in the width of both wave functions is obtained (Fig. 2) as well as the asymmetry forced by the triangular shape of the quantum well (Fig. 1).

For the strong electric field applied across the structure, the initial increase in the electron–hole distance is observed. During the 0.1 ps the electron and hole dynamics is almost independent, although for the electric field weaker than 7×10^7 V/m the exciton is formed. As presented in Fig. 3, the dynamics of the created pair is strongly correlated and the electron and hole wave functions are centered in the same part of the quantum well. A small difference in the position comes from the wave function asymmetry which is a consequence of the different effective mass and is increased by the applied external field. As mentioned before,

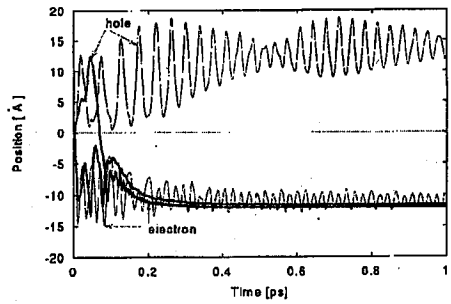

Fig. 3. Electron and hole position for the applied external uniform field 2.57×10^7 V/m (thin line) and 2.57×10^8 V/m (thick line).

for the stronger field, the pair is destroyed and each particle oscillates with the frequency determined by the local triangular potential.

The obtained results allow us to understand the process of creation of the electron–hole pair in the quantum well as well as formation and early time dynamics of the exciton.

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