Excitons in quantum disks and disk arrays

S. GLUTSCH, B. ADOLPH and F. BECHSTEDT

Friedrich-Schiller-Universität, Institut für Festkörpertheorie und Theoretische Optik, Max-Wien-Platz 1, 07743 Jena, Germany

We present a theory which describes the influence of the Coulomb attraction on the optical spectra for quantum dots within the envelope function formalism. Starting from a generalized non-local Elliott formula absorption and luminescence spectra are traced back to two-particle wave functions and energies. They are solutions of the corresponding Schrödinger equation for interacting electron-hole pairs in confinement potentials determined by the spatial variation of the band edges of the considered microstructure. A complete numerical analysis of the two-particle problem for flat quantum dots, i. e. disks for which the size quantization in z -direction is much stronger than that in the xy -plane is presented.

1. INTRODUCTION

Novel crystal growth techniques together with nanometer lithographic techniques have made it possible to fabricate various semiconductor microstructures among them quasi-0D quantum dot systems. One interesting preparation technique is the focussed-laser-beam-induced thermal cation interdiffusion of narrow quantum-well structures [1], whereby the form of the written laser lines determines the lateral shape of the resulting flat microstructure.

The spectroscopy of optical interband transitions across the band gap is a powerful tool to study these systems. This holds particularly for the photoluminescence. The corresponding spectra are governed by efficient intrinsic radiation of free excitons. Studying the development of the excitonic line spectra one can learn somewhat about the mutual interaction of excited electrons (e) and holes (h) and its interplay with the vertical and lateral confinement potentials.

2. BASIC EQUATIONS

For systems, for which the spatial variation of the photon propagator may be neglected, the optical properties can be expressed in terms of a frequency-dependent optical susceptibility $\chi(\omega)$. With the matrix element $|\mu|$ of the underlying dipole-allowed optical transition the optical susceptibility

can be rewritten as a sum over oscillators

$$\chi(\omega) = \frac{2}{\epsilon_0 V} |\mu|^2 \sum_{\beta} \frac{f_{\beta}}{E_{\beta} - \hbar(\omega + i\Gamma_{\beta})} \quad \text{with} \quad f_{\beta} = \left| \int d^2\mathbf{R} \Phi_{\beta}(\mathbf{R}, 0) \right|^2. \quad (1)$$

In the quasi-0D case expression (1) replaces the Elliott formula well known for the 3D and 2D cases. The optical function is directly related to the electron-hole pair wave functions $\Phi_{\beta}(\mathbf{R}, \mathbf{r})$ and energies E_{β} with β as the complete set of quantum numbers for the two-particle problem. According to the preparation method described in Ref. 1 we assume strong confinement in growth (i. e. z -)direction. Therefore its sufficient to study only the most interesting spectral region of the first heavy-hole-to-conduction band transition. As a result, the pair equation can be rewritten for motions in the xy -plane with the 2D Coulomb potential $v(\mathbf{r}) = -e^2/(4\pi\epsilon_0\epsilon z_0)\sinh(z_0/r)$, where z_0 is the width of the underlying quantum-well structure and ϵ stands for the relative static dielectric constant of the semiconductor representing the disk material.

Using center-of-mass (cm) and relative (rel) coordinates $\mathbf{R}, \mathbf{r}$ and E_g^{2D} as the energetical distance of first heavy-hole and first electron well subband, the Schrödinger equation for the pair motion in the xy -plane follows to be

$$\left\{ E_g^{2D} - \frac{\hbar^2}{2M_0} \nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2m_0} \nabla_{\mathbf{r}}^2 + W_e(\mathbf{R} + \frac{m_h}{M_0}\mathbf{r}) + W_h(\mathbf{R} - \frac{m_e}{M_0}\mathbf{r}) + v(\mathbf{r}) \right\} \Phi_{\beta}(\mathbf{R}, \mathbf{r}) = E_{\beta} \Phi_{\beta}(\mathbf{R}, \mathbf{r}). \quad (2)$$

The excitons are considered to be optically excited in flat cylindrical quantum dots of characteristic lateral radius r_0 , usually consisting of GaAs and embedded in a semiconductor layer with a higher energy gap (usually $\text{Ga}_{1-x}\text{Al}_x\text{As}$), which itself is incorporated between barrier layers. The Al mole fraction x as a function of the distance from the disk center is responsible for the electron and hole confinement potentials in the xy -plane. In order to model the effect of the finite disk barriers we describe isolated disks by potentials of the forms

$$W_i(r_i) = \Delta E_i [1 - \exp(-(r_i/r_0)^2)] \quad (i = e, h). \quad (3)$$

with ΔE_i as the corresponding band discontinuities. A profitable result of such a potential choice is the unique splitting of the electron and hole confinement potentials into confining potentials for the center-of-mass motion, the relative motion, and a coupling term of the two motions. The exact solutions of the equation (2) may be expanded in terms of functions obtained without coupling

$$\Phi_{\beta}(\mathbf{R}, \mathbf{r}) = \sum_{N,n} \sum_{M,m} c_{Mm}^{\beta}(N, n) \Psi_{NM}(R) \psi_{nm}(r) \frac{1}{2\pi} e^{i(M\Phi + m\varphi)}, \quad (4)$$

where the radial parts with certain radial quantum numbers N and n as well as eigenvalues E_{NM} and ϵ_{nm} obey decoupled Schrödinger equations. We solve them by means of a Raileigh-Ritz-Galerkin method [2] successfully used already in the case of quantum wires [3]. The unknown coefficients $c_{Mm}^{\beta}(N, n)$ are derived from a system of algebraic equations which results from Eq. (2) with the ansatz in Eq. (4).

3. RESULTS

Figs. 1 and 2 shows the imaginary part of the optical susceptibility (4) near the energy gap E_g^{2D} between the first electron heavy-hole subband in the underlying quantum well structure. For numerical reasons a small line broadening $\hbar\Gamma = 0.05E_B$ is assumed independent of the certain two-particle state. The spectra are plotted for different disk radii r_0 and the confinement potentials in

(3). In Fig. 1 a nearly infinite barrier potentials is used, the quantum well thickness is neglected (i. e. $z_0 \rightarrow 0$), and no overlap of wave functions localized in different disks is taken into account. For large dots Fig. 1(a) the excitonic spectrum of the underlying GaAs quantum well is reproduced. Decreasing the disk radius Fig. 1(b,c) strong quantization effects in the center-of-mass motion are observed. A series of blue-shifted satellites with smaller oscillator strengths and belonging to higher quantum numbers N appear. In addition a finestructure, related to the influence of the disk confinement on the internal motion of the electron hole pairs, occurs Fig. 1(c). The Coulomb degeneracy is lifted. The coupling of the two motions becomes more and more important for the decreasing dot radii, and for radii close to the Bohr radius Fig. 1(d,e) In this limit the disk confinement leads to well separated peaks, which can be interpreted in terms of uncorrelated electrons and holes, i. e. the physical nature of the spectra changes qualitatively. For very small disks the Coulomb attraction seems to be treated as a small perturbation. To check this assumption optical spectra with and without the Coulomb interaction of electrons and holes are also calculated. Then one can show that for $r_0 \leq a_B$ (a_B - the Bohr radius of the bulk exciton) the peaks mainly arise from uncorrelated electron-hole pairs and are only shifted by the Coulomb attraction. They can be nearly characterized by pairs of single-particle quantum numbers of electrons and holes. On the other hand, the Coulomb correlation strongly increases the oscillator strenghts and the Coulomb shift of the peaks does not follow clear rules.

The effect of the finiteness of the barriers and the overlap, when the lattice constant of the array approaches the disk extent, is rather similar to the findings for finite quantum wires and wire arrays [3]. For not too narrow disk the resulting optical line spectra are very similar over an energy interval of the magnitude of the potential heights. However, in the strong confinement limit, i. e. $r_0 < a_B$, the spectra are not only blue-shifted. The number of spectral lines is reduced since the highest excitation state does not fit energetically in the disk. Moreover, the oscillator strength increases with quantum number as in the case of a parabolic potential. According to the preparation by laser-induced interfussion the most pronounced effect in the case of overlapping disks concerns a blue shift indicating an increase of the effective 2D energy gap E_g^{2D} . The material in the center of the discs changes from GaAs to GaAlAs. The imaginary part of the optical susceptibility Eq. (2) is plotted in Fig. 2 for different effective dot radii r_0 and finite but equal z and $\hbar$ confinement potentials with $\Delta E_i = 10E_B$.

To compare with experimental luminescence results [1] some realistic feature should introduced in the description: A certain occupation factor has to be multiplied. The spectra are cut at the high energy side where no luminescence appear. The damping parameter Γ should dependss on the disk radius because of the thickness fluctuations in the underlying quantum well structure.

- [1] K. Brunner, G. Abstreiter, M. Walther, G. Böhm, and G. Tränkle, Surface Sci. 267, 218 (1992); K. Brunner, U. Bockelmann, G. Abstreiter, M. Walther, G. Böhm, G. Tränkle, and G. Weimann, Phys. Rev. Lett. 69, 3216 (1992).
- [2] J. Stoer and R. Burlisch, Introduction to Numerical Analysis (Springer, New York 1983).
- [3] S. Glutsch and F. Bechstedt, Phys. Rev. B47, 4315 + 6385 (1993).

Fig. 1 Imaginary part of the optical susceptibility for different disc radii and infinite high potential: $r_0 = 50$ (a), 10 (b), 5 (c), 2 (d), and $1 a_B$ (e).

Fig. 2 Imaginary part of the optical susceptibility for different disc radii and finite high potential: $r_0 = 50$ (a), 10 (b), 5 (c), 2 (d), and $1 a_B$ (e).