UDC 530.1

NONLINEAR FRACTALS AND EXCITON FORMATIONS IN NANOSTRUCTURED SEMICONDUCTORS

Z.Zh. Zhanabayev, T.Yu. Grevtseva

Al-Farabi Kazakh National University, Tole bi Street, 96, 050012, Almaty, Kazakhstan, mptl@list.ru

We suggest the fractal model for the description of exciton spectra in amorphous and porous semiconductors. Because of theirs chaotic structure the well-known analogy of exciton with hydrogen-like atom is insufficient.

We obtain equations for energy of exciton, biexciton and trion depending on photon energy. Comparison of results of our theory to the recent experimental data is given in the paper. Theory shows the existence of most universal regularities of dynamical systems.

Keywords: fractal model, exciton , exciton spectra, semiconductors, photon energy.

Introduction

Excitons and exciton formations such as biexcitons and trions can be used for distinguishing quick-changing information signals. So, excitons are the subject of many studies on nanoelectronics. Overlapping of wave functions of electrons and holes is probable in nanoclustered semiconductors. Therefore, exciton binding energy in such semiconductors is greater than in infinitely homogeneous medium. These facts suggest a possibility of generation of excitonic quantum bits at sufficiently great, even at room temperatures.

Generally, due to the specific character of technology processes (implantation, diffusion-limited aggregation) nano-sized semiconductors have irregular, chaotic structure. Here, such semiconductors characterized by fractal regularities though on a small range of scale of measurements. Therefore, properties of excitons can't be described universally via smooth regularities which follow, for example, from differential equations. So, a common analogy between exciton and hydrogen-like atom can't be used for a full description of specifics of excitonic spectra in noncrystalline semiconductors with chaotic structure [1].

Such conclusion follows also from experimental works [2, 3] devoted to the description of some self-similarity, quantum-mechanical coherence and decoherence between an exciton and biexciton. Therefore, we put the natural question whether energy exciton spectra have properties of fractal curves.

The aim of this paper is to develop the new model due to describe nonlinear fractal evolution of excitons in dependence upon stimulating photon energy and comparison of results with available experimental data.

Nonlinear fractal measures

The main properties of fractals are their self-similarity and dependence of measure on scale of measurements. We mean that measure is a physical value which can be characterized by additive measurable set. For example, measures of a geometrical fractal are its length, square and volume. Nanoobjects have surprising variety of physical properties because their measures depend on their values according to nonlinear laws. This fact brings out clearly to necessity of fractal analysis in nanoscience.

By use of well-known theories of fractals we choose minimal scale of measurement (size of cells covering an object) independently on value of defining measure. For the description of evolution of measure in dependence upon given parameter of order which is determining variable of a physical process, we choose the scale of measurement via this parameter and desired measure. Hence, fractal measure is a nonlinear function depending on the process.

The traditional definition of fractal measure M can be written as

$$M = M_0 \left(|\Delta M| / M_* \right)^{-\gamma},\ \gamma = D - d,\ \gamma > 0, \tag{1}$$

where M_0 is a regular (non-fractal) measure, ΔM is a scale of measurements, M_* is norm of M, D is fractal dimension of the set of values of M, d is topological dimension of norm carrier. ΔM is independent on M, therefore, measure defining by (1) can be tentatively called the linear value.

If parameter of order is λ we can choose ΔM as

$$\Delta M_M = \frac{|M-\lambda|}{M} = \left|1-\frac{\lambda}{M}\right|,\ \Delta M_\lambda = \frac{|M-\lambda|}{\lambda} = \left|1-\frac{M}{\lambda}\right|, \tag{2}$$

where indexes M and λ correspond to the norms ΔM. According to (2) we can rewrite the formula (1) as

$$M_M = M_0 \left(\left|1-\frac{\lambda}{M}\right| \right)^{-\gamma},\ M_\lambda = M_0 \left(\left|1-\frac{M}{\lambda}\right| \right)^{-\gamma}. \tag{3}$$

At $\gamma \to 0$ we have $M_M = M_\lambda = M_0$, it corresponds to the meaning of M_0. At $\lambda = 0$ we have $M_M = M_0$, $M_\lambda = 0$. It means that the fractal measure defined by its own norm exists in a case when external influence characterized by parameter λ is absent.

We apply the equation (3) for the description of excitonic spectrum. Let us suppose that we have an electron in conduction band and a hole in valence band in a semiconductor. Band gap is E_g, effective mass of electron is m_e, effective mass of hole is m_h. The rest particles produce a background with dielectric capacitivity ε. We consider that interaction between these two quasi-particles occurs according to Coulomb's law. So, by using Schrödinger equation for hydrogen atom, we can obtain the equation for full energy of electron-hole pair:

$$E_n\left(\vec{k}\right) = E_g + \frac{h^2 k^2}{2\left(m_e + m_h\right)} - \frac{m_e m_h e^4}{2\varepsilon^2 \hbar^2 n^2 \left(m_e + m_h\right)},\ n = 1, 2, 3... \tag{4}$$

We shall not take into account energy of motion of exciton “as a whole”. Thus, exciton quasi-momentum $\vec{k}$ is equal to zero. Let us designate binding energy of electron and hole in exciton (the last term in equation (4)) as E. We shall consider a case of excitation of electron by photon with energy $\hbar w$ sufficient for electron transition to valence band. So, we can rewrite equation (4) as

$$\hbar w - E_g = E. \tag{5}$$

Using new simplified designations $M_M = M = E_1$, $M_0 = E_0$, $\lambda = \hbar w - E_g$, $M_\lambda = E_{1,w}$, from equation (3) we obtain the equation for energy of single exciton E_1:

$$E_1 = E_0 \left(\left|1-\frac{\hbar w - E_g}{E_1}\right| \right)^{-\gamma} \equiv f\left(E_0, E_1\right),\ E_{1,w} = E_{0,w} \left(\left|1-\frac{E_{1,w}}{\hbar w - E_g}\right| \right)^{-\gamma} \equiv f\left(E_{0,w}, E_{1,w}\right). \tag{6}$$

Here E_0 is exciton energy at excitation threshold by photon with $\hbar w = E_g$. In this case $E_{0,w} = 0$.

Biexciton, trions and other clusters can be described via hierarchical structures:

$$E_n = f\left(... f\left(\frac{E_0}{n}, E_n \right) ... \right), \tag{7a}$$

$$E_{n,w} = f\left(... f\left(\frac{E_{0,w}}{n}, E_{n,w} \right) ... \right), n = 1, 2, ..., \tag{7b}$$

where number of brackets is equal to n. Equation (7*a*) corresponds to choosing of scale of measurements of fractal measure relative to the measure and describes evolution of excitons, biexcitons and other structures existing in a ground state, i.e. without of external radiation. Equation (7*b*) corresponds to choosing of scale of measurements of fractal measure relative to photon energy and describes excited states. Equations (6), (7*a*), (7*b*) determines energy of system which consists of exciton formations:

$$E = \sum_{i=1}^{n} E_i, n = 1, 2, ... \tag{8}$$

Here $n = 1$ describes an exciton, $n = 2$ – biexciton, $n = 3$ – trion and so on.

In the simplest case in semiconductors with intrinsic conductivity absorption coefficient is defined via density of number of states which is proportional to the square root of energy:

$$\alpha(w) = const \cdot \sqrt{E} = \alpha_0 \sqrt{E} \,. \tag{9}$$

Coherence and decoherence described in experimental works [2-4]. It is possible to draw a conclusion about presence of coherence by examination of instantaneous phase and corresponding frequency. Instantaneous phase $\varphi(t)$ of a signal $x(t)$ can be described via standard Hilbert transform as

$$\varphi(t) = arctg\left(\frac{x^H(t)}{x(t)}\right), \; x^H(t) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{x(\tau)}{t-\tau} d\tau \,. \tag{10}$$

Mean "frequency" along the intervals of $\hbar w$ is defined as

$$F = \left\langle \left| \frac{d\left|\varphi(\hbar w)\right|}{d(\hbar w)} \right| \right\rangle. \tag{11}$$

Results of the numerical analyses

Let us consider exciton-biexciton spectra described by equations (6)-(8) in nanostructured semiconductor films. Varying the parameters E_g, E_0, γ, it is possible to obtain different types of exciton spectra.

(a) (b)

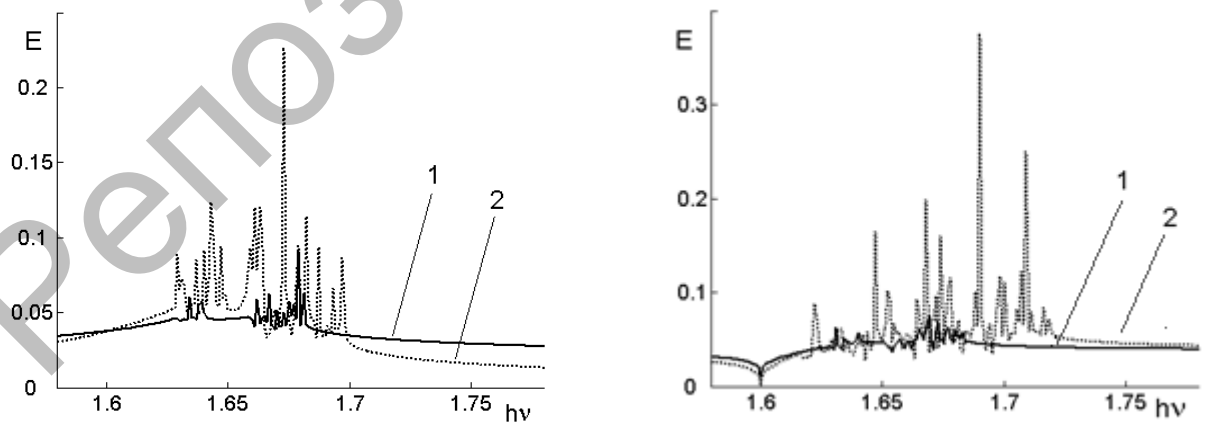

Fig. 1. Influence of parameter γ on the exciton-biexciton spectrum. (a) – equation (7a), (b) – equation (7b): $E_g = 1.6eV$, $E_0 = 0.05eV, 1-\gamma = 1-I_2, 2-\gamma = 1-I_1$.

(a)

(b)

(c)

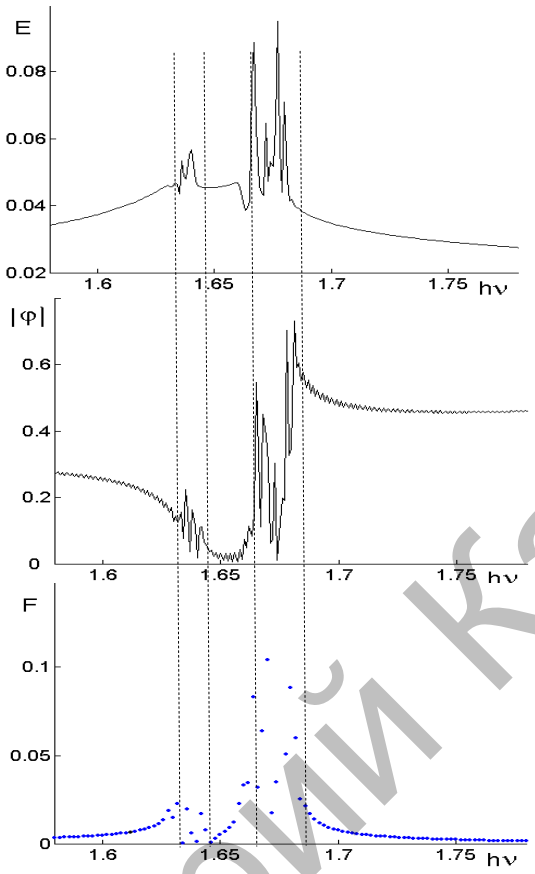

Fig. 2. Exciton-biexciton spectrum (a), module of phase (b) and mean frequency (c): $E_g = 1.6eV$, $E_0 = 0.05eV$, $\gamma = 1 - I_2$.

Fractality leads to increasing of amplitude of oscillations and extending of spectra (Figure 1). We used self-similar $(1-I_2)$ and self-affine $(1-I_1)$ values of fractal dimensions [1]. Increasing of energy gap width E_g leads to the shift of oscillation region towards greater values of photon energy.

We can strictly distinguish regions of exciton and biexciton oscillations (big and small oscillations). It is possible by use of terms "phase - frequency" (Figure 2). It confirmed the presence of coherence. We define coherence as some phase difference between regions of oscillations of exciton and biexciton. Location of peaks and their number inside of these regions depend on γ and number of points used for simulation. Figures 2 were obtained with the step $\Delta\hbar w = 10^{-3}$ eV.

Comparison of theoretical results to experimental data

Figure 3(a) shows exciton-biexciton spectrum of a quantum dot recorded at 4 K [2]. The quantum dot was fabricated on a GaAs(311) substrate by metalorganic vapor epitaxy. The quantum dot is a self-assembled quantum dot. Each peak of photoluminescence (PL) spectrum corresponds to an excited state of exciton or biexciton. Figure 3(b) illustrates the exciton-biexciton spectrum, which was calculated by equations 7(a), (8) and (9).

(a) (b)

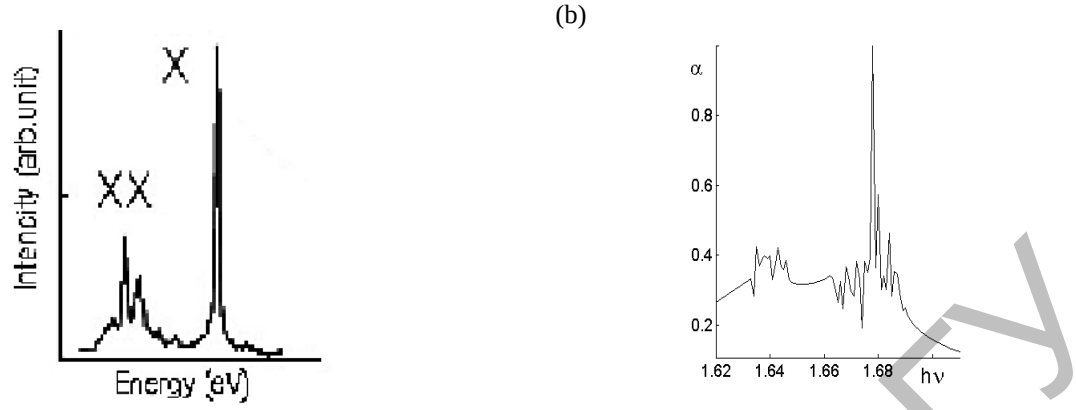

Fig. 3. Exciton-biexciton PL spectrum from an isolated InGaAs quantum dot. Experimental data [2] (a), results of numerical analyses (b): $E_g = 1.6\ eV, \gamma = 0.244,\ E_0 = 0.05\ eV,\ \Delta\hbar w = 10^{-4}\ eV$.

Figure 4(a) shows experimental exciton PL spectrum from InGaAs quantum dots fabricated by metalorganic vapor epitaxy [3]. The sample has two quantum dot layers. Separation between each layer is about 5 nm. Figure 4(b) shows result of simulation by equations 7(a), (8) and (9).

(a) (b)

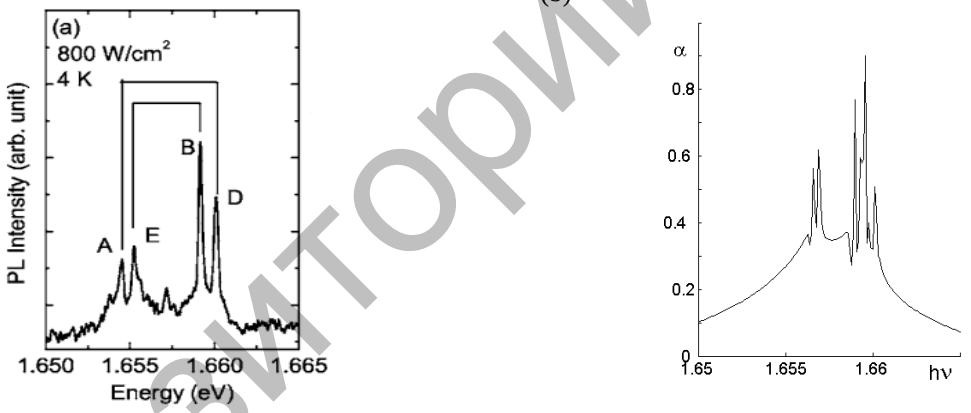

Fig. 4. PL spectrum from bilayer InGaAs quantum dots. Experimental data [3] (a), results of numerical analyses (b): $E_g = 1.65\ eV, \gamma = 1 - I_2,\ \ E_0 = 4 \cdot 10^{-3}\ eV,\ \Delta\hbar w = 10^{-4}\ eV$.

Discussion

Shift of exciton and biexciton spectra by photon frequency is observed in theoretical figures. Exciton peaks in theoretical curves are seen in ranges of $\hbar w \sim 10^{-2} \div 10^{-3}$ eV. These facts correspond to experimental data. If we choose E_0, E_g according to the conditions of experiment, then we have good agreement between theoretical and experimental results. Amplitudes of exciton spectra and spectra of excitonic formations correspond to experimental data. Threshold energy E_0 which need to formation of exciton depends on character of localization of nanostructures and temperature. Meaning of E_0 is maximal phonon energy. Exciton destructed if phonon energy is greater than E_0.

It is worthy of notice that in experiment [2] biexciton forms around of quantum dot. Region of its localization it not limited artificially. Biexciton can be formed between two quantum dots [3].

Distance between quantum dots is about 5 nm, i.e. strong localization stimulates formation of exciton at small E_0. These facts correspond to the theory.

So, fractal model of the dependence of electron-hole pair energy on energy of exciting photon can be used for the description of coherence between exciton formations. The terms "quantum-mechanical coherence" and "coherence of wave processes of different nature" have diverse meanings. Quantum-mechanical coherence means the time interference between wave functions only. It appears as energy oscillations in a system. Generally, coherence means that phase difference is stable by some determining variables at subsystem evolution. In excitonic formations coherence can be observed in these different types.

Conclusions

In the present work we suggest the new equation for fractal measure depending on itself and scale of measurements. This measure correctly describes a hierarchy of excitonic formations. The theory describes conditions for initiation of oscillations and for energy peaks coherence of exciton formations. These new ideas can find wide applications in modern nanoelectronics.

References:

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